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Section A

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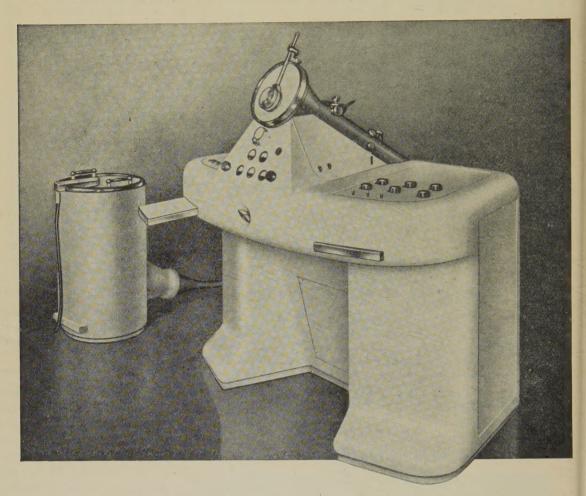
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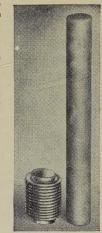
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Section A

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EDITORIAL

Beginning with this issue the *Proceedings* will appear in two Parts, "A" and "B". This change has been dictated by the increasing volume of important communications which has proved too great even for the larger amount of space available since monthly publication began in January 1948.

It is intended provisionally to publish in Part A papers dealing with subjects such as the quantum theory, statistical mechanics, nuclear physics and cosmic rays, atomic physics, molecules, spectra, theories of solids, liquids and gases, surface phenomena, growth and properties of crystals, crystal structure, luminescence, electrodynamics, heat and thermodynamics, and standards. Part B will include subjects such as acoustics (including ultrasonics), optical design, electron optics, colour, elasticity and other mechanical properties of solids and liquids, crystal structure analysis, magnetic materials, refrigeration and liquefaction, electric discharges, radio, geo- and ionosphere physics, astrophysics, and solar physics. It is obvious that a hard and fast dividing line cannot at present be drawn, but we feel sure that in a short time each Part will develop a character of its own, so that the reader will have little difficulty in deciding with which he wishes to be supplied.

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G. Ingle Finch,

President.

Collision Problems and the Theory of Radiation Damping *

By J. HAMILTON

Manchester University

Communicated by L. Rosenfeld; MS. received 12th May 1948

ABSTRACT. The relation between radiation damping theory and the problem of the radiationless collision of an electron with a field of force is discussed. It is shown that the divergence difficulties, such as appear in the damping treatment of Compton scattering do not arise, and the "cut-off" of damping technique is not necessary. The same result applies to the relativistic collision of two electrons.

§ 1. INTRODUCTION AND SUMMARY

Thas been pointed out by Bethe and Oppenheimer (1946) that an uncritical application of the equations developed by Heitler and Peng (1942) for treating radiation damping, leads to incorrect results when applied to the radiationless collision of particles under a static interaction potential. It is, of course, clear that the damping theory was developed in order to treat the interaction of quantized fields with particles to a higher degree of accuracy than is possible by the conventional perturbation theory. It may, however, be of interest to discuss the relation between damping theory and collision problems from a general point of view. This should give some idea of the range of validity of the theory, and some guide as to its application to more complicated problems, such as bremsstrahlung.

The scattering of a particle by a central static field of force is considered in the non-relativistic case. This collision problem is treated by the same method as was used in an earlier paper (Hamilton 1947), to be referred to as I, to deal with the damped scattering of radiation by an electron. Thus it is possible to compare in detail the treatment of the collision problem and of Compton scattering. The equations which describe the change in the free particle system due to the presence of the potential energy can be written in the same form as the equations which connect the initial and final states in the damping theory treatment of Compton scattering. The first difference between the two cases is that infinite transverse self-energy terms have to be neglected in the Compton scattering problem before any reasonable equations connecting the initial and final states can be formulated.

A more important difference arises in the solution of these two sets of equations. In Compton scattering it is essential to limit the energy of the final states to a narrow band of values centred on the energy of the initial state. The excluded final states would give an infinite contribution of such a type that the scattering cross-section would vanish (cf. I, §7(a)). Relativistic invariance is not violated by this procedure, as the breadth of this energy band tends to zero as the size of the enclosing box becomes infinite. If the final states to be considered in the collision problem be limited to a similar narrow band of energies it is shown that a result is obtained which is in agreement with the result got by applying

^{*} This paper forms part of a thesis presented to the University of Manchester for the Ph.D. degree.

the Born approximation, when the latter is valid. When the Born approximation is not valid, this limitation to a narrow band of final energy values is easily seen to be incorrect.

Further investigation of the collision problem shows that those final states which lie outside the narrow energy band do not give an infinite contribution; in fact they give just that contribution which is necessary to lead to the correct collision cross-section as deduced by the phase method. Thus, in general, a direct application of the equations which were developed to treat the damped scattering of radiation leads to results which have no greater accuracy or range of validity than those given by the Born approximation. It seems that, when there is no reason (such as divergency) for the limitation of the range of energy values of the final states, the Heitler-Peng equations, in their simple form, are no longer valid.

In §§ 2-4 the case of a central force of finite range is treated, and in §5 the modifications which are necessary in dealing with the Coulomb potential are indicated. In both these cases it is possible to simplify the calculations by using a simple relation which exists between the phase shift of the wave mechanical method of treating scattering, and the energy shifts which play an important part in the damping phenomenon.

In §6 the relativistic collision of two electrons (without the emission of radiation) is discussed. While the restriction to radiationless collisions makes the discussion of limited validity, it seems that there is no more serious convergence trouble for high energies of the final states when the lowest order relativistic interaction is used, than when the Coulomb interaction alone is used. Thus the parts of the interaction due to longitudinal and transverse photons, respectively, are not treated by different methods, as would be the case if the transverse part had to undergo a cut-off procedure; and the relativistic invariance is not violated.

It would be useful to have a general criterion which would indicate those cases in which it is essential to limit the possible energies of the final states. It is a fact that, so far as the electromagnetic field is concerned, this limitation has only been required in problems in which a change in the free photon configuration is considered (i.e. emission or scattering of a photon). This may be a general rule.

It might be expected from a correspondence principle argument that no damping problem in the usual sense arises in the collision of two electrons. In classical or quantum theory, damping expresses the reaction of the emitted or scattered entity on the emitter or scatterer. In the former, damping takes the form of certain reactive forces, while in the latter it can be regarded as arising from a re-normalization of the wave function of the initial state. The classical theory of electron collisions introduces no damping effect of this nature, and the same may be expected to hold for the non-relativistic quantum theory treatment.

That divergence troubles are absent from the simple treatment of the radiation-less relativistic collision of two electrons is also to be expected. Møller (1931) has shown that the part of the interaction which results from the virtual emission and absorption of one photon, can be regarded as being due to the interaction of the currents which arise from the motion of the electrons. As it is possible to treat the motion of an assembly of charges and currents by the ordinary quantum mechanical methods without any difficulty, it is to be expected that no divergence of energy integrals will arise in the present treatment. It may be of interest

to remember that the relativistic interaction of the electrons can be regarded, by the correspondence principle, as arising from uniformly moving electrons, so that no acceleration of the electrons is involved, and no radiation reaction arises.

These arguments apply to the electromagnetic field only. The interaction of the charges and currents arising from the meson fields of nucleons cannot be treated by the ordinary quantum mechanical methods, and divergence difficulties

are expected to occur in treating collisions involving these particles.

There is, of course, in principle, a distinction between the existence of divergence difficulties and the presence of a damping effect. Even if quantum electrodynamics were well behaved so that no divergent integrals arose, it would be possible to express the damping effects of emitted or scattered radiation. In that case the Heitler-Peng formalism would have to be altered so as to allow for those final states which lay outside the narrow energy band. In view of the above discussion it is possible to go further and state that such a modification would be particularly necessary in cases where the interactions are strong, and the damping is, therefore, really important.

The question of the effect of the emission of radiation on the collision of an electron with a field of force is not considered in the present paper. Bethe and Oppenheimer (1946) applied the Heitler-Peng equations to the *bremsstrahlung* process in which only one photon is emitted, and they found that the infra-red catastrophe appeared in a very troublesome way. As all the final states interact with each other in any damping treatment it is essential that all the physically

important states are considered.

Ferretti and Peierls (1947) pointed out that this imposed a restriction on the validity of Bethe and Oppenheimer's treatment, due to the possible emission of many photons. They showed that for the single photon treatment to be valid, it is essential to enclose the system in a reflecting or periodic box of a size such that $(e^2/hc) \ln (E/p_{\min}) \ll 1$, where p_{\min} is the lowest photon energy allowed by the size of the box, while E is the initial kinetic energy of the electron. Ferretti and Peierls showed that, if the size of the box be such that this condition holds, there is a damping correction to the radiationless scattering cross-section, which depends logarithmically on the linear dimensions of the box. They suggested that this was a meaningless result.

The bremsstrahlung problem has been partially investigated. It has been shown that, in the single photon case, the damping correction to the cross-section for radiationless collisions of the electron is just the total cross-section for collisions in which a photon is emitted. Although this correction does depend on the size of the box in the way Ferretti and Peierls suggest, it clearly has a very reasonable interpretation. A solution of the bremsstrahlung process for the case in which the box may be infinite appears to be very complicated.

§ 2. THE PHASE SHIFT

In this and the two following sections the collision of a particle with a central field of force of finite range is considered. Spherical polar coordinates are the most convenient. In order to show the connection between the phase shift of the wave function of the scattered particle and the change in the energy levels which occurs in going from the free particle system to the system in which the

potential energy acts on the particle, it is essential to enclose the particle in a large spherical box. This box is assumed to be impenetrable; its centre coincides with the centre of force, and its radius is denoted by R.

The motion of a free particle in such a box is given by the wave function

$$\Phi_p(r) = Cr^{-\frac{1}{2}}J_{l+\frac{1}{2}}(pr)Y_{lm}(\theta,\phi),$$
(1)

where J and Y are Bessel functions and spherical harmonics, respectively, and C is a normalizing constant; p is the radial momentum, and \hbar is taken as being unity. The asymptotic form of such a wave function is $\Phi \sim r^{-1} \sin{(pr - l\pi/2)}$. The boundary condition requires $pR - l\pi/2 = n\pi$, where n is an integer. Thus the p values are equally spaced by the amount

$$\Delta p = \pi/R$$
.(2)

This corresponds to an energy spacing, in the non-relativistic case, of $\Delta E = (p/m)(\pi/R)$, where m is the mass of the particle.

When the problem of the scattering of a free particle by the potential energy V(r) is solved by the normal methods, the result can be expressed by the asymptotic form of the wave function, viz. $\Psi \sim r^{-1} \sin{(pr - l\pi/2 + \delta_l)}$. If this scattering takes place within an impenetrable box of radius R a spectrum of p values is selected, given by $p'R - l\pi/2 + \delta_l = n_l\pi$. These new values of the momentum are related to the momentum values of the free particle by the equation

$$(p'-p)R = -\delta_l. \qquad \dots (3)$$

If Λ is the new energy value corresponding to p', and E the original energy, then (2) and (3) give

$$\pi(\Lambda - E)/\Delta E = -\delta_l. \qquad \dots (4)$$

§ 3. THE BORN APPROXIMATION

As the potential V(r) is independent of angles and spin the coupling of the free states (1) which V introduces does not mix the angular momentum quantum numbers l, m. In what follows the case l=0 will be treated. The method of treating damping theory developed in I will be followed, in so far as it is applicable to the scattering problem. Denoting the states of the free particle by the quantum number p, the equations giving the behaviour of the system when V(r) is introduced are (cf. I, eqn. (4))

$$(E_p - \Lambda)A_p + \sum_{p'} H_{pp'}A_{p'} = 0. \qquad (5)$$

 E_p and Λ are the energies of the free and the coupled system respectively, the A_p are the normal amplitude functions, and $H_{pp'} = \int_0^R r^2 dr \, \Phi_p(r) V(r) \Phi_{p'}(r)$. $\Phi_p(r)$ is given by (1) with l=0.

Following the treatment of Compton scattering (I, §6) new amplitude functions are introduced by the relation $V_p = (\Lambda - E_p)A_p$. Substitution in (5) gives

$$V_p = \sum_{p'} H_{pp'} V_{p'} / (\Lambda - E_{p'}).$$
 (6)

If Λ lies in the region between $E_{p''}$ and the next highest energy value, the sum in (6) can be split up, conveniently, into a sum over the 2N values of $E_{p'}$ situated symmetrically about $E_{p''}$, and a sum over the remaining $E_{p'}$ values.

The result of this separation gives

$$V_{p} = \sum_{[2N]} \frac{H_{pp''}V_{p''}}{A - E_{p'}} + \sum_{(Ep'')} \frac{H_{pp'}V_{p'}}{E_{p''} - E_{p'}}, \qquad \dots (7)$$

where [2N] denotes the region about $E_{p''}$, and $(E_{p''})$ the remainder. The details of the transition from (6) to (7) are given in the Appendix.

Equation (7) gives

$$V_{p} = H'_{pp''}V_{p''}\frac{m}{p''}\cot\{(\Lambda - E_{p''})\pi/\Delta E\} + \frac{1}{\pi}\int_{(p'')}\frac{H'_{pp'}}{E_{p''} - E_{p'}}V_{p'}dp', \dots (8)$$

where the second sum in (7) has been replaced by an integral. (p'') indicates

that the principal value has to be used at p' = p'', while $H'_{pp'} = RH_{pp'}$.

According to the damping theory technique for radiation developed in I, the second term on the right hand side of (8) has to be neglected. In the radiation case this term is infinite. Neglecting this term in the present case will lead to the results obtained by indiscriminate application of the Heitler-Peng equations to collision problems.

Thus (8) gives $V_p = H'_{pp''}V_{p''}(m/p'') \cot \{(\Lambda - E_{p''})\pi/\Delta E\}$. Putting p = p'',

it follows that

$$\tan \{(\Lambda - E_{p''})\pi/\Delta E\} = (m/p'')H'_{p''p''}, \qquad \dots (9)$$

or using (4),

$$\tan \delta_0 = -(m/p'')H'_{p''p''}. \qquad \dots (9 a)$$

Allowing for the fact that the normalized functions $\Phi_p(r)$ of (1) have a radial part given by $\Phi_p(r) = (\pi p/R)^{\frac{1}{2}} r^{-\frac{1}{2}} J_{\frac{1}{2}}(pr)$, (9 a) gives

$$\tan \delta_0 = -\frac{1}{2}\pi \frac{8\pi^2 m}{\hbar^2} \int_0^\infty V(r) [J_{\frac{1}{2}}(pr)]^2 r \, dr \qquad \dots (10)$$

on re-introducing \hbar .

This agrees with the usual Born approximation for δ_0 , viz.

$$\delta_0 = -\frac{1}{2}\pi \frac{8\pi^2 m}{\hbar^2} \int_0^\infty V(r) [J_{\frac{1}{2}}(pr)]^2 r \, dr, \qquad \dots (11)$$

which is valid provided $\delta_0 \leq 1$.

It can be seen readily that (10) gives incorrect results if the right hand side is large. Consider a potential V(r) which is extremely strong where r < a, and which vanishes where r > a. Then the true value of δ_0 is approximately -(a/p), but the right hand side of (10) is, in general, certainly not $-\tan(a/p)$.

Thus the technique used for the damping of radiation when applied to a collision problem gives a value for the phase which agrees with that derived by using the Born approximation, in cases where the Born approximation is valid; but it gives an incorrect result in cases where the Born approximation is not valid. It follows that the region of validity of the Heitler-Peng equations for collision problems is the same as that of the Born approximation.

§ 4. THE EXACT SOLUTION

It remains to show that it is possible to take account of the second term on the right hand side of (8), and that this equation then leads to the correct value of the phase.

Equation (8) can be written

$$V_p = \lambda H'_{pp''} V_{p''} + \frac{1}{\pi} \int_{(p'')} \frac{H'_{pp'}}{E_{p''} - E_{p'}} V_{p'} dp', \qquad , \dots (8 a)$$

where λ is an eigenvalue to be determined. H' is independent of R, the radius of the box, and so is $\Phi_p'(r) = R^{\frac{1}{2}}\Phi_p(r)$. Actually $\Phi_p'(r) = \sqrt{2} \sin(pr)/r$. To find the solutions of $(8\,a)$ it is useful to study the properties of the homogeneous integral equation

$$W_p = \mu \int_0^\infty H'_{pp'} W_{p'} dp'. \qquad \dots (12)$$

Equation (12) will have a set of real eigenvalues μ_{α} , and a corresponding set of solutions W_p^{α} . The functions W_p^{α} are orthogonal, and if the α form a discrete set, the W_p^{α} can be normalized so that $\int_0^{\infty} dp' W_{p'}^{\alpha} W_{p'}^{\beta} = \delta_{\alpha\beta}$. Then

$$H'_{pp'} = \sum_{\alpha} W_p^{\alpha} W_{p'}^{\alpha} / \mu_{\alpha}, \qquad \dots (13)$$

where the summation extends over all values of a. However, the definition

$$H'_{pp'} = \int_0^\infty \Phi'_p(r)V(r)\Phi'_{p'}(r)r^2dr,$$
(14)

remembering the orthogonal properties of the $\Phi_p'(r)$, suggests that α denotes the continuous spectrum given by r, and that the W_p^{α} are related to the $\Phi_p(r)$. If $W_p^r = \pi^{-\frac{1}{2}} r \Phi_p'(r) = (2/\pi)^{\frac{1}{2}} \sin(pr)$ then

$$\lim_{P \to \infty} \int_{0}^{P} W_{p}^{r} W_{p}^{r'} dp = \pi^{-1} \lim_{P \to \infty} \left\{ \frac{\sin P(r-r')}{r-r'} - \frac{\sin P(r+r')}{r+r'} \right\} = \delta(r-r')$$
.....(15 a)

where $\delta(r-r')$ is the Dirac δ -function. Similarly, the other orthogonal relation holds, viz.

$$\lim_{R\to\infty} \int_0^R W_p^r W_{p'}^r dr = \delta(p-p'). \qquad \dots (15 b)$$

Now (14) can be written in the form

$$H'_{pp'} = \int_0^\infty \frac{W_p^r W_{p'}^r}{\mu_r} dr,$$
(16)

which is analogous to (13). It follows that $1/\mu_r = \pi V(r)$. It can easily be verified that the W_p^r , μ_r , thus defined are the solutions of equation (12).

To solve (8 a) substitute $V_p = \int_0^\infty dr \ a_r W_p^r$ (i.e. the solution of (8 a) is expanded in terms of the solutions of (12)).

Using (16) and the orthogonality relations (15) this gives

$$\mu_r a_r = \int_0^\infty dr' a_{r'} \{ \lambda(r, r') + [r, r'] \}, \qquad \dots (17)$$

where $(r, r') = W_{p''}^r W_{p''}^{r'}$, $[r, r'] = \frac{1}{\pi} \int_{0^{(p'')}}^{\infty} dp' \frac{W_{p'}^r W_{p'}^{r'}}{E_{p''} - E_{p'}}$. Using $E_p = p^2/2m$ gives

$$[r, r'] = -(2m/\pi p'') \begin{cases} \cos(r'p'') \sin(rp'') & r < r' \\ \sin(r'p'') \cos(rp'') & r > r' \end{cases},$$

and also $(r, r') = (2/\pi) \sin(p''r) \sin(p''r')$. Further, substituting $\alpha_r = \mu a_r$, (17) leads to the equation for α_r

$$\alpha_{r} = 2\{\lambda \sin(p''r) - (m/p'') \cos(p''r)\} \int_{0}^{r} dr' \alpha_{r'} V(r') \sin(p''r') - 2(m/p'') \sin(p''r) \int_{\pi}^{\infty} dr' \alpha_{r'} V(r') \cos(p''r'). \qquad \dots (18)$$

From (18) it follows that if α_r is everywhere finite then $\alpha_0 = 0$. By differentiation of (18) it is readily seen that α_r satisfies the equation

$$d^{2}\alpha_{r}/dr^{2} + \{(p'')^{2} - 2mV(r)\}\alpha_{r} = 0. \qquad (19)$$

As is well known the solution of (19), together with the condition $\alpha_0 = 0$, leads to the asymptotic form for large r

$$\alpha_r \sim A \sin(p''r + \delta_0),$$
(20)

where A tends to a constant as $r \rightarrow \infty$. The asymptotic form of (15), on the other hand, is

$$\alpha_r \sim 2\{\lambda \sin(p''r) - (m/p'')\cos(p''r)\} \int_0^\infty dr' \alpha_{r'} V(r') \sin(p''r'). \qquad \dots (21)$$

Comparing (20) and (21), it follows that $\cot \delta_0 = -\lambda p''/m$.

Thus cot $\delta_0 = -\cot \{(\Lambda - E_{p''})\pi/\Delta E\}$, in agreement with the exact relation (4). Hence the additional term in (8 a) gives a finite correction to the Born approximation—a correction which gives the exact result as deduced by the phase method.

Equation (21) yields the further relation for the phase

$$\sin \delta_0 = -2(m/p'')A^{-1} \int_0^\infty dr \, \psi(r) V(r) \sin(p''r), \qquad \dots (22)$$

where $\psi(r)$ is the finite solution of (19) which has the asymptotic form $\psi \sim A \sin(p''r + \delta_0)$. Equation (22) can be verified by the usual methods.

Finally, it should be noted that the same method could be used for values of l other than zero, with a slightly more complicated analysis.

§ 5. THE COULOMB FIELD

The investigations of the previous sections can be carried through for the Coulomb interaction, with some slight modifications. It is well known that in this case the phase contains an additional factor $(-\ln r)$. This corresponds to the fact that H'_{pp} depends logarithmically on R, the radius of the enclosing sphere. It is therefore necessary to keep the radius R finite, but large. The connection between the phase shift and the energy difference, established in §2, then holds (provided the $\ln R$ term is included as being part of the phase). The p values now form a discrete set, and some integrations are to be replaced by summations.

In the Appendix it is shown that the transition from (6) to (7) can also be made in the Coulomb case. The last term in equation (8) is to be replaced by the summation $\pi^{-1}\Delta p \sum_{p'} (p'')(H'_{pp'})/(E_{p''}-E_{p'})$ where $H'_{pp'}=\int_0^R \Phi'_p(r)V(r)\Phi'_{p'}(r)r^2dr$. Further, (15 a) becomes $\Delta p \sum_p W_p^r W_p^{r'}=\delta(r-r')$. The modified form of (12), $W_p=\mu\Delta p \sum_{p'} H'_{pp'}W_{p'}$ has the solutions W_p^r . Equation (17) can be derived, with the modifications that the upper limit of the integration over r' is now R,

while [r, r'] is given by a summation over the p' values. Equations (18) and (19) follow easily, and (21) is replaced by

$$\alpha_R = 2\{\lambda \sin(p''R) - (m/p'')\cos(p''R)\} \int_0^R dr' \alpha_{r'} V(r')\sin(p''r').$$

From this it again follows that $\cot \delta_0 = -\cot \{(\Lambda - E_{p''})\pi/\Delta E\}$.

It is clear, therefore, that for the Coulomb interaction the damping theory cut-off is no more justified than it is for a static interaction of finite range.

§6. THE RETARDED INTERACTION OF TWO ELECTRONS

The result of the preceding section leads to the question of what part damping plays in the collision of two electrons when the retardation and velocity dependent effects are considered. It might be guessed that as the damping theory was developed for quantized fields, it will modify that part of the interaction which arises from transverse photons. On the other hand, it is difficult to see how such a treatment could avoid destroying the Lorentz invariant form of the total interaction (cf. Møller 1931).

Any investigation of the nature of the corrections to be applied to the first order perturbation method of treating the relativistic scattering of electrons must be mainly formal. Of the two reasons for this, the first is that the correction due to the emission of radiation is of the same order as any correction to Møller's (1932) collision cross-section. The other reason is that the matrix elements are very strongly dependent on the angle of scattering, if the latter is small; so that it is apparently impossible to apply perturbation theory to calculate the higher order corrections.

It is easiest to use a linear momentum representation (and a cubic periodic box). The fundamental equations (5) become

$$(E_c - \Lambda)A_{cl} + \sum_{c'l} H_{cl,c'l'}A_{c'l'} = 0, \qquad \dots (23)$$

where c, c' label the distinct energy levels, while l, l' denote the directions of the momenta and the spins of the two electrons in the initial and final states respectively. $H_{cl,c'l'}$ is the matrix element connecting the states (c, l) and (c', l'), and is composed of the Coulomb interaction matrix element, together with the compound matrix elements arising from the exchange of one transverse photon between the two electrons.

Substituting $(\Lambda - E_c)A_{cl} = V_{cl}$, and changing the summation over l' into an integration, equation (23) can be written as

$$V_{cl} = \pi \lambda \int dl' H_{cl, c'l'} \rho(E_{\bar{c}}l') V_{cl'} + \int_{(E_{\bar{c}})} dE_{\bar{c}'} dl' \frac{H_{cl, c'l'} \rho(E_{c'}l') V_{c'l'}}{E_{\bar{c}} - E_{c'}}, \quad \dots (24)$$

where Λ lies in the vicinity of $E_{\bar{c}}$. $\rho(E_c l)\Delta E_c dl$ is the number of final states in the range $(\Delta E_c, dl)$; ΔE_c is the interval between two discrete energy levels in the neighbourhood of E_c , while $\lambda = \cot \{(\Lambda - E_{\bar{c}})\pi/\Delta E_{\bar{c}}\}$. (In the linear momentum representation there is no simple relation between λ and the phase.)

In the damping theory treatment of Compton scattering the second term on the right hand side of (24) is neglected, because the integration over the energy diverges. It can easily be seen that, in the Compton scattering case, the compound matrix element corresponding to $H_{cl,c'l'}$ behaves like $(E_{c'})^{-\frac{1}{2}}$ as $E_{c'} \rightarrow \infty$.

Suppose that in the problem of the collision of two electrons the initial momenta are \mathbf{p}_a , \mathbf{p}_b ; and the final momenta are \mathbf{p}_a' , \mathbf{p}_b' . Then the Coulomb matrix element is

$$4\pi e^2/[|\mathbf{p}_a - \mathbf{p}'_a|^2], \quad (\hbar = c = 1),$$
(25)

while the term in e² due to the transverse photon field is (Heitler 1944, p. 98)

$$\frac{2\pi}{k}e^{2}\left[\left(\alpha^{a}\alpha^{b}\right) + \frac{(E_{a} - E'_{a})(E_{b} - E'_{b})}{k^{2}}\right]\frac{(E_{a} + E_{b}) - (E'_{a} + E'_{b}) - 2k}{\{E_{a} - E'_{a} - k\}\{E_{b} - E'_{b} - k\}} \quad \dots (26)$$

 E_a , E_b ; E'_a , E'_b are the initial and final energies of the electrons, while $k = |\mathbf{p}_a - \mathbf{p}'_a| = |\mathbf{p}'_b - \mathbf{p}_b|$. Conservation of energy is not assumed in calculating (25) or (26).

For k much larger than p_a , p_b , and the rest mass of the electrons, (26) takes the form $(2\pi e^2/k^2)[\alpha^a\alpha^b)+1]$ and, for very large final energies, $E_c\sim 2k$. It is therefore to be expected that if the matrix element (25) gives no divergence difficulty in the energy integral occurring in equation (24), the same will apply to (26). As it is not permissible to neglect all but a narrow energy band in the case of the Coulomb interaction, it seems unjustified to apply the damping theory cut-off to the interaction given by (26). However, the general remarks on the essentially formal nature of any consideration of (26) at high energies should be remembered.

Finally, it may be noted that substituting the left hand side of (24) in the integral on the right hand side gives

$$\begin{split} V_{\bar{c}l} = \pi \lambda \int dl' \left\{ H_{\bar{c}l,\,\bar{c}l'} + \int_{(E_{\bar{c}})} dE_{c''} \int dl'' \, \frac{H_{\bar{c}l,\,c''l''} \rho(E_{c''}l'') H_{c''l'',\,\bar{c}l'}}{E_{\bar{c}} - E_{c''}} \right\} \rho(E_{\bar{c}}l') V_{\bar{c}l'} \\ + (\text{a term in } H.H.H.). \end{split}$$

Here $\int dE_{e''}$ is a convergent integral, but $\int dl''$ gives rise to an infinity when l'' is parallel to l, or to l' (in the centre of gravity system). Such a substitution method of approximating to (24) is therefore impossible, because of the strong angular dependence of the matrix elements.

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APPENDIX

The transition from equations (6) to (7) for finite range interactions can be justified as follows. Consider first the $(E_{p''})$ region, which is the region remaining when the N terms higher and lower than $E_{p''}$ are excluded.

On $(E_{p''})$ the term $1/(\Lambda - E_{p'})$ can be written

$$\begin{split} \frac{1}{\Lambda - E_{p'}} &= \frac{1}{E_{p''} - E_{p'}} + (\Lambda - E_{p''}) \frac{\partial}{\partial E_{p''}} \left(\frac{1}{E_{p''} - E_{p'}} \right) \\ &\quad + \frac{(\Lambda - E_{p''})^2}{2\,!} \frac{\partial^2}{\partial E_{p''}^2} \left(\frac{1}{E_{p''} - E_{p'}} \right) + \dots \end{split}$$

The order of magnitude of the ratio of the second term on the right hand side to the first is $|(\Lambda-E_{p''})/(E_{p''}-E_{p'})|$; and on $(E_{p''})$ this is less than r/N, where $(\Lambda-E_{p''})/\Delta E=r$, and r=O(1). Choosing $N=KR^{(\frac{1}{2}+\epsilon)}$, where $0<\epsilon<\frac{1}{2}$ and K is a constant, this ratio can be made negligible. Thus the second, and similarly the higher order terms on the right hand side of the series can be neglected compared with the first term. With this definition of N, it follows that $N\Delta E=(\pi p''/m)R^{(\epsilon-\frac{1}{2})}$ tends to zero as $R\to\infty$. Thus the breadth in energy of the region [2N] about $E_{p''}$ which contains the 2N energy levels tends to zero as $R\to\infty$.

For the region [2N] it is convenient to use the expansion

$$H_{pp'}V_{p'} = H_{pp''}V_{p''} + (E_{p'} - E_{p''}) \frac{\partial}{\partial E_{p''}} (H_{pp''}V_{p''}) + \dots$$
 (A)

It is assumed that $H_{pp'}V_{p'}$ does not vary rapidly on [2N]. Further

$$\label{eq:sum_eq} \begin{array}{l} \sum\limits_{[2N]} \frac{E_{p'} - E_{p''}}{\Lambda - E_{p'}} = \\ -2N + (\Lambda - E_{p''}) \sum\limits_{[2N]} \frac{1}{\Lambda - E_{p'}} \, . \end{array}$$

If N, and so R, is sufficiently large, the last term gives

$$\{(\Lambda-E_{p^{\prime\prime}})\pi/\Delta E\}\cot\{(\Lambda-E_{p^{\prime\prime}})\pi/\Delta E\}.$$

It is therefore negligible compared with the term -2N. The first term on the right hand side of (A) gives the first term in (7) whose value is

$$H'_{pp''}V_{p''}(\pi/R\Delta E)\cot\{(\Lambda-E_{p''})\pi/\Delta E\},$$

where $H'_{pp''} = RH_{pp''}$. $H'_{pp''}$ is independent of R provided

$$R \int_{0}^{R} \Phi_{p}(r) V(r) \Phi_{p''}(r) r^{2} dr$$

converges as $R \to \infty$. This is true when V(r) is a potential of finite range. $R\Delta E$ is independent of R. The second term on the right hand side of (A) gives a term in (7)

$$-2N\,\frac{\partial}{\partial E_{n''}}(H_{pp''}V_{p''}) = -\,\frac{2N}{R}\frac{\partial}{\partial E_{n''}}(H'_{pp''}V_{p''}) = O(R^{-\frac{1}{2}+\epsilon}).$$

This can be neglected. Similarly it can be shown that the higher order terms in (A) do not contribute to (7).

When V(r) is of the form 1/r it is essential to keep R finite, but it can be seen that by choosing R sufficiently large, the errors involved in going from (6) to (7) can be made as small as is desired.

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Damping Theory and the Propagation of Radiation*

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ABSTRACT. It is shown that a careful examination of the concepts involved in radiation damping theory makes it possible to treat the propagation of energy from one atom to another through the electromagnetic field. An exact and continuous solution of the propagation problem is given.

§ 1. INTRODUCTION AND SUMMARY

It has been suggested by Ferretti and Peierls (1947) that the quantum theory of radiation damping leads to incorrect results when it is applied to a problem which involves the propagation of radiation. They consider the resonance interaction of two atoms through the medium of the electromagnetic field; and they suggest that a consequence of the damping theory is that energy is propagated from one atom to the other at a velocity other than the velocity of light. They reach this conclusion after making use of the ideas of "roundabout transitions" and "intermediate" states which are involved in the application of damping theory to the scattering of radiation (Heitler and Peng 1942). The present paper is an attempt to show that there need be no difficulty in the propagation problem, provided these ideas are examined carefully; and, in addition, it is an attempt to obtain an exact solution for this problem.

It is assumed that there are two identical atoms A and B, which can interact by emitting and absorbing photons. For simplicity the states considered are: two, in which one atom is in its excited state and the other is in its normal state; and an infinity, in which both atoms are in their normal states and one photon is present. For such a system there need be no confusion due to "roundabout transitions". This type of transition can be defined as involving the emission and re-absorption of the same photon by the same electron, and it is clear that such a transition leads to an infinite self-energy term in the solution. No such transition arises in the simple treatment of the propagation problem. Having excluded these roundabout transitions, it is obvious that, if two distinct transitions lead from an observable initial state to an observable final state, there is no reason to neglect one of them.

The idea of "intermediate" states in the damping theory requires more detailed examination. The concept first arose in the treatment of the intermediate states occurring in Compton scattering. Those states have an energy which differs by a finite amount from the energy of the initial state for the scattering problem. Moreover, the energy spread of the final states tends to zero, as the enclosing "periodic" box becomes infinite; so the intermediate states cannot have the same energy as any of the final states. For scattering problems, therefore, the intermediate states are not observable; they have a mathematical meaning only. As a consequence, in the damping theory solution of scattering, the

^{*} This paper forms parts of a thesis presented to the University of Manchester for the Ph.D. degree.

possibility of the energy of the coupled system of particle and radiation being equal to the energy of an intermediate state is neglected. Further, in normalizing the total probability to unity, the possibility of the system being found in any intermediate state is neglected.

The intermediate states (states in which one photon is present and both atoms are unexcited) which may occur in the propagation problem are of quite different nature from those which have just been discussed. Any of the intermediate states in the propagation problem may be observed; so they are no more intermediate than they are final states. That they happen to be coupled to final states of another kind is incidental. Further, it is clear that they have to be considered in normalizing the total probability; and it will appear from the detailed solution that they give the major contribution to the normalization equation. There is, therefore, no basis for treating these states by the same method as was used for the intermediate states in the scattering problem.

It is shown that these considerations lead to a reasonable result for the propagation problem. The method of discrete energy levels developed in an earlier paper (Hamilton 1947), to be referred to as I, is used, and the treatment of the simple atomic emitter is followed closely. The presence of the second atom causes a splitting of the energy levels of the interacting system, a splitting which is inversely proportional to the separation of the atoms. This splitting makes it possible for the second atom to remain in its ground state for the correct time after the first atom starts radiating.

On the basis of Weisskopf and Wigner's solution for the atomic emitter, Kikuchi (1930) has shown that the electromagnetic disturbance which is emitted travels with the velocity of light. Wentzel (1933) shows in a similar manner how the propagation problem can be treated. The present solution differs from these in that the reaction of the second atom on the first is considered, and that the solution obtained for the excitation probability of the second atom is a continuous function of the time. Both the above authors make substitutions for the excitation of the second atom which are discontinuous in time.

§ 2. THE FUNDAMENTAL EQUATIONS

The system composed of two identical atoms A and B and any radiation is enclosed in a large cubic "periodic" box. It will be assumed that each atom has only one excited state, and states in which more than one photon occurs will be neglected. As was shown in I, the unperturbed states of such a system have a discrete energy spectrum; and it can be assumed that the distinct energy levels (which are highly degenerate) are equally spaced.

The unperturbed states to be considered are: (0) atom A excited and no photon present, (1) atom B excited and no photon present, (i) both atoms in their normal state and a photon "i" present. 0, 1, i, will be used to label these states. The effect of the coupling between the atoms and the radiation field can be expressed by the equations (cf. I, eqn. (11))

$$(E_{0}-\Lambda)A_{0} + \sum_{i} H_{0i}A_{i} = 0,$$

$$(E_{i}-\Lambda)A_{i} + H_{i0}A_{0} + H_{i1}A_{1} = 0,$$

$$(E_{1}-\Lambda)A_{1} + \sum_{i} H_{1i}A_{1} = 0.$$

$$(1)$$

The E denote the energies of the uncoupled states, the H are the usual matrix elements for emission and absorption of radiation, and the A are the amplitude factors describing the coupled states; Λ is the energy value of the coupled system. Different solutions of the set (1) will be denoted by the index μ .

Following I, any state of the coupled system can be described by the wave function Ψ , which can be written in the form $\Psi = \sum c_{\mu} \Psi^{\mu}$ where the c_{μ} are constants depending on the initial conditions and $\Psi^{\mu} = \sum_{r}^{\mu} A_{r}^{\mu} \exp{\{-i(\Lambda_{\mu} - E_{r})t\}} \psi_{r}$. The index r runs over 0, 1 and all the i, while the ψ_{r} are the wave functions of the uncoupled system. Ψ can also be written

$$\Psi = \sum_{r} a_r \psi_r, \qquad \dots (2)$$

where $a_r(t) = \sum_{\mu} A_r^{\mu} \exp \left\{ -i(\Lambda_{\mu} - E_r)t \right\}$ is time dependent. If the initial conditions are

$$a_0(0) = 1,$$
 $a_1(0) = 0,$ $a_i(0) = 0,$ (2')

then $c_{\mu} = \overline{A_0^{\mu}}$.

Due to the positions of atoms A and B being different (both atoms are regarded as being massive and immovable), the matrix elements H_{0i} , H_{1i} are not identical. They are related thus

 $H_{1i} = \exp\{i(\mathbf{p}_i \cdot \mathbf{r}')\}H_{0i}, \qquad \dots (3)$

where \mathbf{r}' is the displacement vector of B relative to A and \mathbf{p}_i is the momentum of photon "i" ($\hbar = c = 1$ throughout).

Elimination of the A_i from (1) gives

$$\begin{split} &\left\{E_{0}-\Lambda+\sum_{\mathbf{i}}\frac{|H_{0\mathbf{i}}|^{2}}{\Lambda-E_{\mathbf{i}}}\right\}A_{0}+\sum_{\mathbf{i}}\frac{H_{0\mathbf{i}}H_{\mathbf{i}\mathbf{1}}}{\Lambda-E_{\mathbf{i}}}A_{\mathbf{1}}=0,\\ &\left\{E_{1}-\Lambda+\sum_{\mathbf{i}}\frac{|H_{1\mathbf{i}}|^{2}}{\Lambda-E_{\mathbf{i}}}\right\}A_{1}+\sum_{\mathbf{i}}\frac{H_{1\mathbf{i}}H_{\mathbf{i}\mathbf{0}}}{\Lambda-E_{\mathbf{i}}}A_{\mathbf{0}}=0. \end{split} \right\} \end{split}$$

Taking $E_0 = E_1$, these equations give

$$(E_1 - \Lambda)^2 + (E_1 - \Lambda)\sum_{i} \frac{|H_{1i}|^2}{\Lambda - E_i} + \sum_{i} \sum_{j} \frac{\{|H_{0i}|^2 |H_{1j}|^2 - H_{0i}H_{1i}\overline{H}_{0j}H_{j1}\}}{(\Lambda - E_i)(\Lambda - E_j)} = 0, \quad \dots (4)$$

where the bar denotes the complex conjugate.

Using (3), any term of numerator of the last summation in (4) becomes $|H_{0i}|^2|H_{0j}|^2$. $[1-\exp\{-i(\mathbf{p_i}\cdot\mathbf{r'})\}]$. The summation Σ in (4) can be split up into a summation over the discrete energy levels, denoted by Σ , and a summation over all the states belonging to a fixed value of E, denoted by Σ .

Consider, for simplicity, that the excited state of either atom is a *p*-state with the magnetic quantum number zero. Then

$$H_{0i} = \text{const.} \int g(r)(z/r) \exp \{i(\mathbf{p}_i \cdot \mathbf{x})\} f(r) dV,$$

with an obvious notation. Thus for dipole radiation

$$H_{0i} = ip_{iz}$$
. const. $\int g(r)f(r)(z^2/r) dV$,

where p_{iz} is the z-component of \mathbf{p}_i . Hence

$$|H_{0i}|^2 = (p_{iz})^2 C$$
,

where C is independent of \mathbf{p}_i .

Denoting the angle between the axis OZ and \mathbf{r}' by θ' , the angular summation of the term containing the exponential factor gives

$$\sum_{\substack{[E_{\mathbf{i}}]\\[E_{\mathbf{i}}]}} \exp\left\{-i(\mathbf{p}_{\mathbf{i}}\cdot\mathbf{r}')\right\} |H_{0\mathbf{i}}|^2 = |\overline{H_{0\mathbf{i}}}|^2 \cdot \left\{\frac{\sin\alpha}{\alpha} + (3\cos^2\theta' - 1)\left(\frac{\sin\alpha}{\alpha} + 3\frac{\cos\alpha}{\alpha^2} - 3\frac{\sin\alpha}{\alpha^3}\right)\right\},\,$$

where $|\overline{H_{0i}}|^2 = \sum_{[E_i]} |H_{0i}|^2$ is the summation of $|H_{0i}|^2$ over all angles, and $\alpha = |\mathbf{p}_i|r'$.

If the zero of energy is taken as the energy of either of the atoms in its normal state, then $|\mathbf{p}_i| = E_i$.

It is convenient to write the angular summation in the form

$$\sum_{[E_{\rm i}]} \exp\left\{-i(\mathbf{p}_{\rm i}\cdot\mathbf{r}')\right\} |H_{0\rm i}|^2 = |H_{0\rm i}|^2 \left\{G_1(E_{\rm i}r')\sin(E_{\rm i}r') + G_2(E_{\rm i}r')\cos(E_{\rm i}r')\right\},$$

where

$$G_1(E_ir') = 3\cos^2\theta'/(E_ir') - 3(3\cos^2\theta' - 1)/(E_ir')^3; \quad G_2(E_ir') = 3(3\cos^2\theta' - 1)/(E_ir')^2.$$

Then

$$\sum_{[E_{i}]} \sum_{[E_{j}]} |H_{0i}|^{2} |H_{0j}|^{2} \left[1 - \exp\left\{-i(\mathbf{p}_{i} \cdot \mathbf{r}')\right\} \exp\left\{i(\mathbf{p}_{j} \cdot \mathbf{r}')\right\}\right] \\
= \overline{|H_{0i}|^{2}} \cdot \overline{|H_{0j}|^{2}} \cdot \left\{1 - \left[G_{1}(E_{i}r')\sin\left(E_{i}r'\right) + G_{2}(E_{i}r')\cos\left(E_{i}r'\right)\right] \\
\times \left[G_{1}(E_{i}r')\sin\left(E_{i}r'\right) + G_{2}(E_{i}r')\cos\left(E_{i}r'\right)\right]\right\}. \quad \dots (5)$$

§ 3. THE ENERGY SUMMATION AND THE EIGENVALUE EQUATION

Assuming that the matrix elements H_{0i} vary slowly with the energy E_i in the important region (i.e. over the ordinary line width) it is possible to separate off energy summations in equation (4) of the type $\sum_{E_i} 1/(\Lambda - E_i)$. Assuming that the

distinct energy levels E_i are equally spaced in the vicinity of Λ such a summation gives

$$\sum_{E_i} 1/(\Lambda - E_i) = (\pi/\Delta E) \cot \{(\Lambda - E_s)\pi/\Delta E\} + \sigma, \qquad \dots (6)$$

where ΔE is the spacing of the energy values, and $E_{\rm s}$ is one of the energy values $E_{\rm i}$ which lies close to Λ . σ is a correction arising from the $E_{\rm i}$ values which lie far from Λ . As the range of $E_{\rm i}$ values centred about Λ over which the summation is made is increased, σ is zero at first, and only becomes appreciable for ranges which are very many times greater than the line width of one of the atoms. Over such large ranges the matrix elements will vary appreciably with $E_{\rm i}$, and (6) would have to be modified. In the extreme case of an infinite range of $E_{\rm i}$ values the term σ leads to the usual transverse self-energy of the bound electron. It is sufficient here to note that in the present problem σ can be neglected for ranges of $E_{\rm i}$ which are many multiples of the line width. Such a limitation will be used in what follows. Under similar conditions

$$\sum_{E_{\rm i}} \frac{\sin{(\Lambda - E_{\rm i})r'}}{\Lambda - E_{\rm i}} = \pi/\Delta E \; ; \quad \sum_{E_{\rm i}} \frac{\cos{(\Lambda - E_{\rm i})r'}}{\Lambda - E_{\rm i}} = (\pi/\Delta E)\cot{\{(\Lambda - E_{\rm s})\pi/\Delta E\}}. \label{eq:energy}$$

The variation of $G_1(E_ir')$, $G_2(E_ir')$ with E_i in the energy summations occurring in (4) can be neglected, provided the "periodic box" is sufficiently large. These functions are therefore replaced by $G_1(\Lambda r')$, $G_2(\Lambda r')$ respectively.

Using these summations, (4) with the aid of (5) reduces to a quadratic equation

for $(\pi/\Delta E)$. $\overline{|H_{0i}|^2}$. $\cot\{(\Lambda - E_s)\pi/\Delta E\}$ whose roots are

$$(\Gamma/2) \cot \{(\Lambda - E_{\rm s})\pi/\Delta E\} = \frac{\Lambda - E_1 \mp \{G_2(\Lambda r')\sin(\Lambda r') - G_1(\Lambda r')\cos(\Lambda r')\} \cdot (\Gamma/2)}{1 \pm \{G_1(\Lambda r')\sin(\Lambda r') + G_2(\Lambda r')\cos(\Lambda r')\}},$$
.....(7)

where the upper or lower signs are to be taken together, and $\Gamma/2 = (\pi/\Delta E) \cdot |\overline{H_{0i}}|^2$. Γ is the ordinary line breadth of either atom (cf. I, §5). According to (7) there will be two roots Λ lying in the energy range ΔE between each two adjacent distinct values of E_i . As $r' \to \infty$ equation (7) becomes

$$(\Gamma/2)\cot\{(\Lambda-E_s)\pi/\Delta E\} = \Lambda - E_1, \qquad \dots (7')$$

which is the eigenvalue equation for the photon emission of one atom. By the definition of the functions G it follows that

$$G_1(\Lambda r') \sim (1/\Lambda r') O(1), \qquad G_2(\Lambda r') \sim (1/\Lambda r')^2 O(1),$$

provided $\Lambda r' \geqslant 1$. O(1) denotes a constant of the order of magnitude unity. Thus the roots of (7) differ from the roots of (7') by amounts of the order of $\Lambda E/(\Lambda r')$, provided $\Lambda r' \geqslant 1$. As $1/\Lambda r' \simeq \lambda/r'$, where λ is the wavelength of the resonant radiation, this condition can be written as $r' \geqslant \lambda$.

§ 4. NORMALIZATION

The condition that the total probability of the system being in all configurations is unity, gives

$$|A_0^{\mu}|^2 + |A_1^{\mu}|^2 + \sum |A_i^{\mu}|^2 = 1$$
(8)

for all values of the root index μ . Substituting from (1) gives

$${A_1}^{\mu}\!=\left\{\! {\scriptstyle \sum\limits_{\rm i}} \! \frac{H_{1{\rm i}} H_{{\rm i}0}}{\Lambda_{\mu}\!-\!E_{\rm i}} A_0 \!+\! {\scriptstyle \sum\limits_{\rm i}} \! \frac{|H_{1{\rm i}}|^2}{\Lambda\!-\!E_{\rm i}} A_1^{\;\mu} \! \right\} . \frac{1}{\Lambda_{\mu}\!-\!E_1} \, . \label{eq:A1}$$

Making these summations by the method of §3, and using (7) to evaluate $\cot \{(\Lambda - E_{\rm s})\pi/\Delta E\}$ where necessary, it appears that

$$A_1^{\mu} = \pm A_0^{\mu}, \qquad \dots (9)$$

where the \pm sign is to be taken according as the upper or lower set of signs is used in (7). Further, from (1), (3) and (9)

$$\begin{split} & \sum_{\mathbf{i}} |A_{\mathbf{i}}^{\mu}|^{2} = |A_{0}^{\mu}|^{2} \cdot \sum_{\mathbf{i}} |H_{0\mathbf{i}}|^{2} \cdot |1 \pm \exp\{-i(\mathbf{p}_{\mathbf{i}} \cdot \mathbf{r}')\}|^{2} / (\Lambda - E_{\mathbf{i}})^{2} \\ & = 2|A_{0}^{\mu}|^{2} \cdot |\overline{H_{0\mathbf{i}}}|^{2} \cdot (\pi/\Delta E)^{2} \cdot \csc^{2}\{(\Lambda - E_{\mathbf{s}})\pi/\Delta E\} \\ & \times \{1 \pm [G_{\mathbf{i}}(\Lambda r')\sin(\Lambda r') + G_{\mathbf{i}}(\Lambda r')\cos(\Lambda r')]\}, & \dots (10) \end{split}$$

provided $r' \ll L$, the linear dimension of the enclosing box.

Now it is clear, by using the relation $\Gamma/2 = (\pi/\Delta E) \cdot |\overline{H_{0i}}|^2$, that in (8) the terms $|A_0^{\mu}|^2$, $|A_1^{\mu}|^2$ are unimportant, as $\pi/\Delta E$ is very large. The normalization is therefore determined by the photon states. From (10) and (7) it follows that

$$|A_0^{\mu}|^2 = \frac{1}{2} \cdot \frac{\overline{|H_{0i}|^2} \cdot \{1 \pm [G_1 \sin(\Lambda r') + G_2 \cos(\Lambda r')]\}}{\{\Lambda - E_1 \mp (\Gamma/2)[G_2 \sin(\Lambda r') - G_1 \cos(\Lambda r')]\}^2 + (\Gamma/2)^2 \{1 \pm [G_1 \sin(\Lambda r') + G_2 \cos(\Lambda r')]\}^2 + \dots (11)$$

§ 5. THE EXCITATION OF THE ATOMS

It follows from (2) that the probability of the occupation of the state ψ_0 is given by $|a_0|^2$, where a_0 is related to the A_0^{μ} through the equation

$$a_0 = \sum_{\mu} c_{\mu} A_0^{\mu} \exp\{-i(\Lambda_{\mu} - E_0)t\}.$$

For the initial conditions (2') $c^{\mu} = \overline{A}_0^{\mu}$, so

$$a_0(t) \exp\{-iE_0t\} = \sum_{\mu} |A_0^{\mu}|^2 \exp\{-i\Lambda^{\mu}t\},$$
(12)

where the summation runs over all the roots of (1). Using (11) it is seen that the summation over the pair of Λ_{μ} values which lie in each energy interval ΔE just cancels out the terms of order λ/r' , leaving a large term, plus terms of order $(\lambda/r')^2$. (The slight difference between the two values of Λ_{μ} give corrections which vanish as $L \to \infty$). Omitting the terms of order $(\lambda/r')^2$ the sum of such pairs of $|A_0^{\mu}|^2$ values is $(|A_0^{\mu}|^2)' = |\overline{H_{0i}}|^2/\{(\Lambda - E_0)^2 + \Gamma^2/4\}$; $(|A_0^{\mu}|^2)'$ is identical with the term $|A_0^{\mu}|^2$ which arises in the single atom problem (cf. I). Replacing the summation in (12) by an integration it is readily seen that $|a_0(t)|^2 = \exp(-\Gamma t)$ as for the single atom.

The behaviour of the probability function $|a_1|^2$ for the excitation of atom B is quite different. This function is given by

$$a_1(t) \exp\left(-iE_1 t\right) = \sum_{\mu} A_1^{\mu} \overline{A_0}^{\mu} \exp\left(-i\Lambda_{\mu} t\right). \tag{13}$$

Relation (9) causes a cancellation of the largest term in $|A_0^{\mu}|^2$, on adding the contribution from the pair of values within a range ΔE . The remaining terms are smaller than $(|A_0^{\mu}|^2)'$ by a factor of the order λ/r' .

Equation (13) can be written in the form

$$a_1 \exp(-iE_1 t) = \sum_{\mu_+} |A_0^{\mu_+}|^2 \exp(-i\Lambda_{\mu_+} t) - \sum_{\mu_-} |A_0^{\mu_-}|^2 \exp(-i\Lambda_{\mu_-} t), \quad \dots (14)$$

where the +, - indicate the two types of roots corresponding to $A_1^{\mu} = \pm A_0^{\mu}$. Also, (11) can be written

$$\begin{split} |A_0^{\mu}|^2 &= \frac{\Delta E}{4\pi i} \left\{ \frac{1}{(\Lambda_{\mu} - E_1 - i\Gamma/2) \pm (\Gamma/2)(G_1 - iG_2) \exp{(-i\Lambda_{\mu}r')}} \right. \\ &\left. - \frac{1}{(\Lambda_{\mu} - E_1 + i\Gamma/2) \pm (\Gamma/2)(G_1 + iG_2) \exp{(i\Lambda_{\mu}r')}} \right\}. \end{split}$$

It can be assumed that $\Lambda_{\mu+} = \Lambda_{\mu-} = \Lambda$, as the error introduced thereby is negligible. Replacing the summation in (14) by an integration gives

$$a_{1} \exp\left(-iE_{1}t\right) = \frac{1}{2\pi i} \left(\frac{\Gamma}{2}\right) \left\{ \int_{-\infty}^{+\infty} d\Lambda \frac{(G_{1} + iG_{2}) \exp\left\{i\Lambda(r' - t)\right\}}{(\Lambda - E_{1} + i\Gamma/2)^{2} - (\Gamma/2)^{2}(G_{1} + iG_{2})^{2} \exp\left(2i\Lambda r'\right)} - \int_{-\infty}^{-\infty} d\Lambda \frac{(G_{1} - iG_{2}) \exp\left\{-i\Lambda(r' + t)\right\}}{(\Lambda - E_{1} - i\Gamma/2)^{2} - (\Gamma/2)^{2}(G_{1} - iG_{2})^{2} \exp\left(-2i\Lambda r'\right)} \cdot \dots (15)$$

Equation (15) is exact, provided the dimensions of the "periodic box" are great enough; and this equation could be used to calculate a_1 to any power of (λ/r') . Here it will be considered sufficient to find a_1 to the lowest power of (λ/r') . Thus G_2 is neglected. Further, the variation of $G_1(\Lambda r')$ with Λ is neglected for the range of values of Λ which is important; and from (15) it is clear that this range is of the order of Γ .

With these assumptions the integrals in (15) can be evaluated by contour integration. The circuit consists of the real axis, together with half of the circle at infinity. On the circle at infinity the second integrand takes the form $\exp{\{y(r'+t)\}/(R^2+C\exp{(2yr')})}$, where $\Lambda=x+iy$, $|\Lambda|=R$, and |C| is a constant. On the half circle y<0 this integrand will give no contribution, provided t>-r'. Moreover, the poles of the second integrand all lie on the half plane y>0. To see this, substitute $\Lambda'=\Lambda-E_1-i\Gamma/2$. The poles are given by

$$\Lambda' = \pm (\Gamma/2)G_1 \exp \{(\Gamma/2)r' - i(E_1 + \Lambda')r'\}.$$

If $\Lambda' = x' - iy'$, this gives

$$\sqrt{(x'^2+y'^2)} = (\Gamma/2)|G_1|\exp\{(\Gamma/2-y')r'\}.$$

As $|G_1| \leqslant 1$, $y' > \Gamma/2$ is impossible, and hence the result. Thus the second integrand gives no contribution to a_1 , provided t > -r'. Actually it represents the "incoming" wave and plays no part in the solution for t > 0.

It is readily seen that the roots of the denominator of the first integrand all lie on the half plane y < 0. On the infinite circle the form of this integrand is $\exp \{-y(r'-t)\}/\{R^2 + C \exp(-2yr')\}$. When t < r' this gives no contribution when integrated over the upper half circle, so $a_1(t) = 0$ if t < r'.

For $t \ge r'$ the value of the integral can be found by noting that, as there are no roots of the denominator on the upper half plane, the integral is equal to

$$-G_1\!\!\int_C\!d\Lambda\,\frac{\exp\left\{i\Lambda(r'-t)\right\}}{(\Lambda-E_1+i\Gamma/2)^2-(\Gamma/2)^2G_1{}^2\exp\left(2i\Lambda r'\right)},$$

where C is the upper half circle at infinity. On C the second term in the denominator can be neglected, giving $-G_1\int_C d\Lambda \left[\exp\left\{i\Lambda(r'-t)\right\}\right]/(\Lambda-E_1+i\Gamma/2)^2$. The path C can be closed by including the lower half circle at infinity which gives no contribution when $t \geqslant r'$. Thus the integral becomes

$$-G_1\int_{\Omega}d\Lambda\left[\exp\left\{i\Lambda(r'-t)\right\}\right]/(\Lambda-E_1+i\Gamma/2)^2$$
,

where O is any contour surrounding the point $(E_1 - i\Gamma/2)$. Hence

$$a_1(t)\exp\left(-iE_1t\right)=iG_1.\left(\Gamma/2\right)(t-r')\exp\left\{-\Gamma(t-r')/2\right\}\exp\left(iE_2r'\right) \qquad (t>r'),$$
 and as $|G_1|^2=K(\lambda/r')^2$, where K is of the order of magnitude unity, the final

result is $|a_1(t)|^2 = 0$ $t \le r'$

$$|a_1(t)|^2 = 0 t \le r' |a_1(t)|^2 = K(\lambda/r')^2 \{\Gamma(t-r')/2\}^2 \exp\{-\Gamma(t-r')\} t > r'$$

Thus the atom B remains in its normal state till time r', after which it is excited for a time of the order $1/\Gamma$. The maximum probability of excitation is of the form $K(\lambda/r')^2$, which is in agreement with the usual ideas on electromagnetic propagation.

The resonance phenomenon will arise from the re-emission of radiation by the atom B, and its absorption by A. The excitation amplitude of A will be of the order $(\lambda/r')^2$, and therefore does not occur in the approximation used in this section.

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Continuous y-Emission in Neutron-Proton Collisions

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ABSTRACT. The cross-section for Bremsstrahlung in neutron-proton collisions is calculated with a central exchange-force model and for energies up to 20 MeV. Its value is found to lie between 10^{-28} and 10^{-29} cm². This probably is too small to be measured with experimental techniques at present available.

§ 1. INTRODUCTION

HE aim of this paper is to estimate the magnitude of the cross-section for Bremsstrahlung in n-p (neutron-proton) collisions and its sensitivity to variation of the hypotheses concerning the n-p interaction. Neutron and proton will be treated here as point particles interacting by means of a central force of the exchange type. Their interaction with radiation will be supposed to conform to the usual theory for particles in a radiation field. We thus omit refinements which have been included by Pais (1943) in his treatment of the photodisintegration of the deuteron.

This simple model is inadequate when the incident neutron energies are high (of the order of the meson rest-energy). Our discussion will thus be restricted to a lower energy-range. The relevant energies will then, in general, not be large compared with a suitable average of the potential. In these circumstances, use of the Born approximation may result in appreciable error. For this reason, exact continuum wave functions of the n-p system will be used to calculate the required cross-sections.

§ 2. WAVE FUNCTIONS

Referred to the centre of gravity frame, (C-system), the wave equation for the internal motion of the n-p system is

$$[\nabla^2 + (M/\hbar^2)(E - V)]\psi(\mathbf{r}; m_1, m_2) = 0.$$
 (2.1)

Here $\mathbf{r} = (x, y, z)$ is the position-vector of the neutron relative to the proton, m_1 and m_2 are spin-variables of the particles, M the mass of a nucleon and 2E is the kinetic energy of the incident neutron in the laboratory system. The interaction operator V will be chosen to represent a mixture of central exchange forces of Majorana and Heisenberg type (cf. Bethe and Bacher 1936, §§ 11, 12, 13).

The wave functions will be required to represent "incoming" or "outgoing" particles which have, at large distances, a definite momentum $\hbar \mathbf{k}$. Correspondingly we determine the following types of solution of (2.1):

(a) To represent incoming particles: solutions which have, for $r \to \infty$, the asymptotic form

 $[\exp\{i(\mathbf{k} \cdot \mathbf{r})\} + \text{diverging spherical wave}] \times (\text{spin function})$

(b) To represent outgoing particles we choose, for reasons of symmetry, those solutions which have the asymptotic form

 $[\exp\{i(\mathbf{k} \cdot \mathbf{r})\} + \text{converging spherical wave}] \times (\text{spin function}).$

The eigenstates can be classified into triplet states with wave functions

$$\psi^{(3)} = U^{(3)}(\mathbf{r})^3 \chi_m \qquad (m = 0, \pm 1), \qquad \dots (2.2)$$

and singlet states with wave functions

$$\psi^{(1)} = U^{(1)}(\mathbf{r})^{1}\chi.$$
 (2.3)

 $^3\chi_m$, $(m=0,\pm 1)$ and $^1\chi$ are the usual normalized symmetric and antisymmetric spin functions of the two-particle problem. The wave equations for triplet and for singlet states are independent. Also, the space part $U^{(3)}(\mathbf{r})$ of the triplet wave function (2.2) is independent of m. On separating out the spin-dependence, the functions $U^{(3)}$ and $U^{(1)}$ satisfy equations which may be written together in the form

$$(\hbar^2 \Delta/M + E) U(\mathbf{r}) = V(r) U(-\mathbf{r}). \tag{2.4}$$

If M(r) and H(r) describe the dependence on distance of the Majorana and Heisenberg potentials, respectively, then

$$V(r) = \left\{ \begin{array}{ll} M(r) + H(r) & \text{(triplet states)} \\ M(r) - H(r) & \text{(singlet states)} \end{array} \right\}. \qquad (2.5)$$

Each wave function will be characterized by an associated wave vector \mathbf{k} of length $k = (ME/\hbar^2)^{\frac{1}{2}}$. This dependence on the parameter \mathbf{k} will be indicated by the notation $U(\mathbf{r}; \mathbf{k})$. Introducing spherical polar coordinates (r, θ, ϕ) with polar axis in the direction \mathbf{k} , those wave functions which satisfy conditions (a) or (b) above can be expanded in the form:

$$U_{\pm}(\mathbf{r}; \mathbf{k}) = \sum_{l=0}^{\infty} (2l+1)i^{l} \exp\{\pm i\eta_{l}(k)\} \frac{u_{l}(r; k)}{kr} P_{l}(\cos \theta) \qquad \dots (2.6)$$

(cf. Mott and Massey 1933). The $P_l(t)$ are non-normalized Legendre polynomials and $u_l(r; k)$ is that solution of

$$\frac{d^2u}{dr^2} + \left[k^2 - \frac{l(l+1)}{r^2} - (-1)^l \frac{MV(r)}{\hbar^2}\right] u = 0 \qquad \dots (2.7)$$

which vanishes for r=0 and which has, for $r\to\infty$, the asymptotic form

$$u_l(r; k) \sim \sin \left[kr - \frac{1}{2}l\pi + \eta_l(k)\right].$$
(2.8)

 U_{+} and U_{-} correspond respectively to the cases with diverging and converging spherical waves.

The incident beam will be assumed to be unpolarized and to consist of particles with wave vector \mathbf{k}_0 (in the C-system). There are then four independent initial states of equal weight:

$$\psi_{\text{in}}(\mathbf{r}; \mathbf{k}_0) = \begin{cases} U_{+}^{(3)}(\mathbf{r}; \mathbf{k}_0)^3 \chi_m, & (m=0, \pm 1) \\ U_{+}^{(1)}(\mathbf{r}; \mathbf{k}_0)^1 \chi & & \end{cases}. \quad(2.9)$$

 $U_{+}^{(3)}$ and $U_{-}^{(1)}$ are given by (2.6) with $\mathbf{k} = \mathbf{k}_0$. Similarly, there are four independent wave functions corresponding to final states with wave vector \mathbf{k} :

$$\psi_{\text{fin}}(\mathbf{r}; \mathbf{k}) = \left\{ \begin{array}{ll} U_{-}^{(3)}(\mathbf{r}; \mathbf{k})^{.3} \chi_{m}, & (m=0, \pm 1) \\ U_{-}^{(1)}(\mathbf{r}; \mathbf{k})^{.1} \chi & \end{array} \right\}, \quad \dots (2.10)$$

 $U_{-}^{(3)}$ and $U_{-}^{(1)}$ are given by (2.6) with **k** as polar axis. (Since V contains no spin-orbit coupling terms, the spin functions in both (2.9) and (2.10) may be referred

to the same coordinate system with \mathbf{k}_0 as z-axis.) We shall denote coordinates in a system with \mathbf{k}_0 as z-axis by (x, y, z) or (r, θ, ϕ) and polar coordinates in a system with \mathbf{k} as polar axis by (r, θ', ϕ') .

Each of the functions in (2.9), (2.10) is normalized per unit volume, i.e.

$$\lim_{v\to\infty}\frac{1}{v}\int_v|U|^2d\tau=1.$$

§ 3. MATRIX ELEMENTS

We shall consider processes in which the n-p system (referred to the C-frame), makes a radiative transition from one of the states characterized by wave vector \mathbf{k}_0 (energy E_0) to states characterized by wave vector \mathbf{k} (energy E). The circular frequency ω of the photon emitted is then given by

$$\hbar\omega = E_0 - E = (\hbar^2/M)(k_0^2 - k^2).$$
 (3.1)

Strictly speaking, the C-systems appropriate to initial and to final states are not identical. The difference—due to the momentum carried off by the photon—is, however, very small and will be neglected.

Two types of process will be taken into account. These are (Bethe and Bacher 1936, §§ 16, 17): (a) transitions induced by the electric dipole $\frac{1}{2}e\mathbf{r}$; and (b) transitions induced by the magnetic dipole $\mu_0\mathbf{T} = \mu_0(\mu_p\mathbf{\sigma}_p + \mu_n\mathbf{\sigma}_n)$, $\mathbf{\sigma}_p$, $\mathbf{\sigma}_n$ are the spin operators and μ_p , μ_n the magnitudes of the magnetic moments in units of a nuclear magneton $\mu_0 = e\hbar/2Mc$.

Correspondingly, we shall have to evaluate matrix elements of the following two main types:

$$\mathcal{M} = \frac{1}{2}e\mathbf{M} = \frac{1}{2}e\int \psi_{\text{fin}}^*(\mathbf{r}; \mathbf{k})\mathbf{r}\psi_{\text{in}}(\mathbf{r}; \mathbf{k}_0)d\tau, \qquad (3.2)$$

$$\mathcal{N} = \mu_0 \mathbf{N} = \mu_0 \int \psi_{\text{fin}}^*(\mathbf{r}; \mathbf{k}) \mathbf{T} \psi_{\text{in}}(\mathbf{r}; \mathbf{k}_0) d\tau. \qquad (3.3)$$

The required cross-sections are to be obtained by calculating the eight partial cross-sections with each of the states (2.9) as initial state and then adding them with weight-factor $\frac{1}{4}$ for each.

Considering first transitions of type (a), the only non-vanishing matrix elements are:

(i) three equal elements:

$$\mathbf{M}^{(3)} = \int U_{+}^{(3)}(\mathbf{r}; \mathbf{k}_{0})\mathbf{r}U_{-}^{(3)*}(\mathbf{r}; \mathbf{k}) d\tau, \qquad \dots (3.4)$$

corresponding to transitions $U_{+}^{(3)}$. ${}^{3}\chi_{m} \rightarrow U_{-}^{(3)}$. ${}^{3}\chi_{m}$, $(m=0, \pm 1)$, and

(ii) one element:

$$\mathbf{M}^{(1)} = \int U_{+}^{(1)}(\mathbf{r}; \mathbf{k}_{0}) \mathbf{r} U_{-}^{(1)*}(\mathbf{r}; \mathbf{k}) d\tau, \qquad (3.5)$$

corresponding to the transition $U_{+}^{(1)} \chi \rightarrow U_{-}^{(1)} \chi$.

In the sum for the composite cross-section, (3.4) contributes with weight $\frac{3}{4}$ and (3.5) with weight $\frac{1}{4}$.

Let (λ, μ) be the angular coordinates of **k** in the coordinate system with \mathbf{k}_0 as polar axis. For conciseness we write

$$\eta_l^{(i)} = \eta_l^{(i)}(k), \quad \overline{\eta}_l^{(i)} = \eta_l^{(i)}(k_0), \quad (i=3 \text{ or } 1)$$
(3.6)

and

$$G_{l,n} = \frac{1}{k_0 k} \int_0^\infty u_l(r; k_0) u_n(r; k) r dr.$$
 (3.7)

In (3.7) $G_{l,n}^{(3)}$ and $G_{l,n}^{(1)}$ are to be distinguished according as triplet or singlet wave

functions and phases are involved.

As it stands, the integral in (3.7) is divergent. However, it is summable, e.g. by inserting a convergence factor e^{-br} and then proceeding to the limit $b \rightarrow 0$ after the integration has been performed. It is in this sense that (3.7) and the analogous divergent integrals in (3.13) have to be interpreted here.

When the wave functions in the form (2.6) are substituted in (3.4) and (3.5) the integrals over angles are easily evaluated by using the spherical harmonic

addition theorem. We find (writing $t \equiv \cos \lambda$)

$$M_z = 4\pi i \sum_{l=0}^{\infty} (l+1) \{ G_{l+1, l} \exp \{ i(\bar{\eta}_{l+1} + \eta_l) \} P_l(t) - G_{l, l+1} \exp \{ i(\bar{\eta}_l + \eta_{l+1}) \} P_{l+1}(t) \},$$
.....(3.8)

$$\begin{split} M_x \pm i M_y &= -4\pi \exp\big(\pm i\mu\big) \sum_{l=0}^{\infty} \big\{ G_{l+1,l} \exp\big\{ i(\bar{\eta}_{l+1} + \eta_l) \big\} P_l^1(t) \\ &+ G_{l,l+1} \exp\big\{ i(\bar{\eta}_l + \eta_{l+1}) \big\} P_{l+1}^1(t) \big\}. \qquad \dots (3.9) \end{split}$$

Turning now to the photomagnetic transitions, the only surviving elements $\mathcal{N}(\mathbf{k}_0; \mathbf{k})$ are of the forms:

 $\mathcal{N}^{(3,1)}$ corresponding to transitions triplet \rightarrow singlet, $\mathcal{N}^{(1,3)}$ corresponding to transitions singlet \rightarrow triplet.

Writing

$$A^{(i,j)} = \int U_{+}^{(i)}(\mathbf{r}; \mathbf{k}_0) U^{(j)*}(\mathbf{r}; \mathbf{k}) d\tau \qquad [(i,j) = (3,1) \text{ or } (1,3)], \quad \dots (3.10)$$

we have

$$\sum_{\text{(3)-states}} \{ |N_x^{(i,j)}|^2 + |N_y^{(i,j)}|^2 \} = 2 \sum_{\text{(3)-states}} |N_z^{(i,j)}|^2 = 2(\mu_{\text{p}} - \mu_{\text{n}})^2 |A^{(i,j)}|^2. \quad \dots \quad (3.11)$$

The cross-sections obtained from (3.11) with (i,j) = (3,1) and (1,3) each contribute with weight $\frac{1}{4}$ to the final cross-section.

Substituting wave functions of the form (2.6) in (3.10) we find analogously to (3.8), (3.9):

$$A^{(i,j)} = 4\pi \sum_{l=0}^{\infty} (2l+1)K_l^{(i,j)} \exp\{i(\bar{\eta}_l^{(i)} + \eta_l^{(j)})\}P_l(t), \qquad \dots (3.12)$$

with

$$K_{l}^{(i,j)} = \frac{1}{k_0 k} \int_{0}^{\infty} u_{l}^{(i)}(r; k_0) u_{l}^{(j)}(r; k) dr. \qquad (3.13)$$

§ 4. CROSS-SECTION FORMULAE

Each wave function (2.9) for an initial state corresponds to an incident current of $2\hbar k_0/M$ neutrons/cm²/second. Each final wave function (2.10) is normalized per unit volume; there are then $(Mk/16\pi^3\hbar^2)dEd\Omega$ final states of each type corresponding to motion within $d\Omega = \sin \lambda d\lambda d\mu$ and with energy in the range (E, E + dE). The factor

$$\frac{M^2}{32\pi^3\hbar^3} \left(\frac{E}{E_0}\right)^{\frac{1}{2}} dE d\Omega \qquad \qquad \dots (4.1)$$

is thus required to translate transition probabilities calculated with the wave functions (2.9), (2.10) into differential cross-sections.

Let $\sigma(E_0; E, \lambda, \alpha) \sin \lambda \sin \alpha \, d\lambda \, d\alpha$ be the cross-section for a process in which (i) the n-p system makes a radiative transition from a state (\mathbf{k}_0, E_0) to a state with energy in (E, E+dE) and direction of motion making an angle between λ and $\lambda + d\lambda$ with \mathbf{k}_0 ; (ii) a photon with circular frequency $\omega = (E_0 - E)/\hbar$ is emitted in a direction making an angle between α and $\alpha + d\alpha$ with \mathbf{k}_0 . Then

$$\sigma(E_0; E, \lambda, \alpha) = \frac{M^2}{32\pi^3 \hbar^3} \left(\frac{E}{E_0}\right)^{\frac{1}{2}} \frac{\omega^3}{\hbar c^3} \{ (|\mathcal{M}_x|^2 + |\mathcal{M}_y|^2)(1 + \cos^2 \alpha) + 2|\mathcal{M}_z|^2 \sin^2 \alpha \}, \dots (4.2)^{\frac{1}{2}}$$

where \mathcal{M} is to be interpreted as $\mathcal{M}^{(3)}$ or $\mathcal{M}^{(1)}$ in the electric dipole case and as $\mathcal{N}^{(3,1)}$ or $\mathcal{N}^{(1,3)}$ in the magnetic dipole case. The corresponding cross-sections will be distinguished by affixing the same indices to σ .

Further cross-sections of interest are derived from (4.2) by integration. They may be written in an obvious notation as $\sigma(E_0; E, \lambda)$, $\sigma(E_0; E; \alpha)$, $\sigma(E_0; E)$ and $\sigma(E_0)$. In particular

$$\sigma(E_0; E) = \frac{M^2 \omega^3}{12\pi^2 \hbar^4 c^3} \left(\frac{E}{E_0}\right)^{\frac{1}{2}} \int_{0}^{\pi} \sum_{x, y, z} |\mathcal{M}_x|^2 \sin \lambda \, d\lambda. \qquad \dots (4.3)$$

From (4.3) with (3.8), (3.9) and with (3.11), (3.12) we have

$$\sigma_{\rm el}^{(i)}(E_0; E) = \frac{2e^2M^2\omega^3}{3\hbar^4c^3} \left(\frac{E}{E_0}\right)^{\frac{1}{2}} \sum_{l=0}^{\infty} (l+1)\{(G_{l,l+1}^{(i)})^2 + (G_{l+1,l}^{(i)})^2\}, \qquad \dots (4.4)$$

$$\sigma_{\text{mag}}^{(i,j)}(E_0; E) = \frac{8\mu_0^2(\mu_p - \mu_n)^2 M^2 \omega^3}{\hbar^4 c^3} \left(\frac{E}{E_0}\right)^{\frac{1}{2}} \sum_{l=0}^{\infty} (2l+1)(K_l^{(i,j)})^2. \qquad \dots (4.5)$$

§ 5. SHORT-RANGE FORCES

For further progress it is necessary to introduce explicit assumptions for the interaction function V(r) in (2.4), (2.7). In this section we assume only that the forces are of short range, so that we may put effectively

$$V(r) = 0$$
 for $r > a$. $\dots (5.1)$

In the range r>a, the required solution of (2.7) can be expressed in terms of Hankel functions:

$$u_{l}(r; k) = \frac{1}{2} \left(\frac{\pi k r}{2} \right)^{\frac{1}{2}} \left\{ \exp\left(i\eta_{l}\right) H_{l+\frac{1}{2}}^{(1)}(kr) + \exp\left(-i\eta_{l}\right) H_{l+\frac{1}{2}}^{(2)}(kr) \right\}. \tag{5.2}$$

The phase $\eta_l(k)$ is determined by fitting the interior and exterior solutions smoothly at r=a; it depends on the detailed form of V(r) in (0,a). (5.2) can also be represented in the form

$$u_l(r; k) = F_l(kr)\sin(kr + \eta_l) + G_l(kr)\cos(kr + \eta_l). \qquad \dots (5.3)$$

 $F_l(x)$ and $G_l(x)$ are polynomials in x^{-1} , defined through the Bessel functions by $(\frac{1}{2}\pi x)^{\frac{1}{2}}J_{l+\frac{1}{2}}(x) = F_l(x)\sin x + G_l(x)\cos x$.

Now, the hypothesis of short-range forces implies that, given k, there exists an integer $l_0(k)$ such that for all $l \ge l_0$, (i) $\eta_l(k)$ does not differ appreciably from zero, and (ii) the $u_l(r; k)$ do not differ appreciably from the unmodified plane-wave components $(\pi k r/2)^{\frac{1}{2}} J_{l+\frac{1}{2}}(kr)$ in the whole range $(0, \infty)$. It follows that, for $l, n \ge l_0(k_0)$, the $G_{l,n}$ in (3.7) can effectively be taken equal to 0. Similar considerations apply to the K_l .

We now introduce the approximation of replacing the integrations over $(0, \infty)$ in (3.7) and (3.13) by integrations over (a, ∞) . This approximation is valid only for energies which are not too high; this has been checked for the case of a rectangular potential (cf. §7). For energies much larger than those considered here the contribution from (0, a) is no longer negligible; the calculated cross-sections would then depend more intimately on the detailed form of V(r) than in the low-energy case.

The integrals for $G_{l, l+1}$ and K_l are now easily evaluated by elementary methods. (The evaluation for higher l can be simplified by using for the u_l certain recurrence formulae analogous to, and easily derivable from, those for the Hankel functions.)

In particular we have

$$(k_0^2 - k^2)^2 G_{0,1} = \left(\frac{E_0}{E} - 3\right) \bar{c}_0 s_1 + 2\left(\frac{E}{E_0}\right)^{\frac{1}{2}} \bar{s}_0 c_1 - k_0 a \left(1 - \frac{E}{E_0}\right) \left[\left(\frac{E_0}{E}\right)^{\frac{1}{2}} \bar{c}_0 c_1 + \bar{s}_0 s_1\right],$$

$$\dots \dots (5.4)$$

$$(k_0^2 - k^2)G_{1,0} = \left(\frac{E}{E_0} - 3\right)c_0s_1 + 2\left(\frac{E_0}{E}\right)^{\frac{1}{2}}s_0\bar{c}_1 + k_0a\left(1 - \frac{E}{E_0}\right)\left[c_0\bar{c}_1 + \left(\frac{E_0}{E}\right)^{\frac{1}{2}}s_0\bar{s}_1\right],$$
.....(5.5)

where, for conciseness, we have written (cf. (3.6))

$$\bar{s}_l \equiv \bar{s}_l^{(i)} = \sin(k_0 a + \bar{\eta}_l^{(i)}), \quad s_l \equiv s_l^{(i)} = \sin(k a + \eta_l^{(i)}), \text{ etc.} \quad \dots (5.6)$$

Also

$$(k_0^2 - k^2)^{3/2} K_0^{(3,1)} = \left(1 - \frac{E}{E_0}\right)^{\frac{1}{2}} \left[\left(\frac{E_0}{E}\right)^{\frac{1}{2}} \bar{c}_0^{(3)} s_0^{(1)} - \bar{s}_0^{(3)} c_0^{(1)} \right], \qquad \dots (5.7)$$

$$(k_0^2 - k^2)^{3/2} K_0^{(1,3)} = \left(1 - \frac{E}{E_0}\right)^{\frac{1}{2}} \left[\left(\frac{E_0}{E}\right)^{\frac{1}{2}} \bar{c}_0^{(1)} s_0^{(3)} - \bar{s}_0^{(1)} c_0^{(3)} \right]. \tag{5.8}$$

§ 6. FORCES OF "ZERO RANGE"

We consider the simple limiting case where the range $a \to 0$. Here $\eta_l^{(i)} \to 0$ for all l > 0. Let ϵ_3 and $-\epsilon_1$ be the binding energies of the deuteron for the ground state and for the virtual singlet level respectively. Then

$$ka + \eta_0^{(3)} \rightarrow \frac{1}{2}\pi + \arctan(\epsilon_3/E)^{\frac{1}{2}}; \qquad ka + \eta_0^{(1)} \rightarrow \frac{1}{2}\pi - \arctan(\epsilon_1/E)^{\frac{1}{2}}. \qquad (6.1)$$

In this case $G_{l,\,l+1},\,G_{l+1,\,l}$ and the K_l are zero for all $l{
eq}0$ and

$$(k_0^2 - k^2)^2 G_{0,1} = 2 \left(\frac{E}{\epsilon + E_0} \right)^{\frac{1}{4}}; \qquad (k_0^2 - k^2)^2 G_{1,0} = 2 \left(\frac{E_0}{\epsilon + E} \right)^{\frac{1}{2}}, \quad \dots (6.2)$$

 ϵ being taken as ϵ_3 for the $G^{(3)}$ and as ϵ_1 for the $G^{(1)}$. Also

$$(k_0^2 - k^2)^{3/2} K_0^{(i,j)} = (\epsilon_3^{\frac{1}{2}} + \epsilon_1^{\frac{1}{2}}) \left[\frac{E_0 - E}{(\epsilon_i + E_0)(\epsilon_i + E)} \right]^{\frac{1}{2}}. \qquad \dots (6.3)$$

The various cross-sections are then given by

$$\sigma_{\rm el}^{(i)}(E_0; E) = \frac{2 \cdot 13 \times 10^{-30}}{E_0 - E} \left(\frac{E}{E_0}\right)^{\frac{1}{2}} \left\{\frac{4E}{\epsilon_i + E_0} + \frac{4E_0}{\epsilon_i + E}\right\}, \quad \dots (6.4)$$

$$\sigma_{\text{mag}}^{(i,j)}(E_0; E) = 1.63 \times 10^{-31} \left(\frac{E}{E_0}\right)^{\frac{1}{2}} (\epsilon_3^{\frac{1}{2}} + \epsilon_1^{\frac{1}{2}})^2 \frac{E_0 - E}{(\epsilon_i + E_0)(\epsilon_j + E)}. \quad \dots (6.5)$$

Table 1 lists total cross-sections (integrated over E) for the various types of process, and total averaged cross-sections $\overline{\sigma}(E_0)$, for a few values of E_0 . The integral for $\sigma_{\rm el}(E_0)$ diverges logarithmically at E_0 ; we have taken

$$\sigma_{\rm el}(E_0) \equiv \int_0^{f^2 E_0} \sigma(E_0; E) dE.$$

The calculation has been made with $\epsilon_3 = 2.17$, $\epsilon_1 = 0.05$ MeV. in (6.4), (6.5) and with $f^2 = 0.95$.

Table 1. Total Cross-sections in Units of 10^{-29} cm² for Radiative Scattering by Protons of Neutrons with Energy $2E_0$ MeV.

E_0 (MeV.)	$\sigma_{\mathrm{el}}^{(3)}$	$\sigma_{ m el}^{(1)}$	$\sigma_{ m mag}$	$\overline{\sigma}(E_0)$
1	1.19	. 3.26	0.02	1.7
4	2.64	4.30	0.05	3.1
6	3.07	4.50	0.06	3.5
10	3.56	4.67	0.08	3.9

§7. FINITE RANGE

The cross-sections were also calculated for energy $E_0=10$ MeV. using a rectangular potential model with range $a=2\cdot 5\times 10^{-13}$ cm., $(V)_{r< a}=25$ MeV. (triplet states), 15 MeV. (singlet states). By far the largest contribution is again due to the electric dipole transitions $l=0 \rightleftharpoons l=1$. The approximation of replacing integrations over $(0,\infty)$ by ones over (a,∞) (cf. § 5) was checked for this case. In no case did the neglected contribution from (0,a) amount to more than 10% of the total; in general it is considerably less, as also is its averaged contribution. In Table 2 are listed the cross-sections for a number of values of E (column 2). For comparison, $\sigma(10,E)$ in the limiting case a=0 are given in column 3.

Table 2. Partial Cross-sections in Units of 10^{-29} cm² for Radiative Scattering by Protons of Neutrons with Initial Energy 20 MeV.

<i>E</i> (Mev.)	$\sigma(10, E)$	$\sigma(10, E), (a=0)$	$\sigma(10, E)$, (max)
1	1.7	1.3	26
5	2.7	2.3	18
7	4.7	4.2	29
9	. 15.0.	13.8	

We have noted that the major contributions to the cross-section, for initial energies E_0 up to about 10 MeV., arises from the terms in $G_{0,1}$ and $G_{1,0}$ of $\sigma_{\rm el}$. For such energies $G_{0,1}$ and $G_{1,0}$ are closely approximated to by (5.4) and (5.5) irrespective of the detailed form of V(r) in (0,a). We thus obtain an upper limit to these coefficients, and so to the calculated cross-sections, by replacing all sine and cosine factors by unity. Then

$$|(k_0^2 - k^2)^2| |G_{0,1}| \le \left| \frac{E_0}{E} - 3 \right| + 2\left(\frac{E}{E_0}\right)^{\frac{1}{2}} + k_0 a \left(1 - \frac{E}{E_0}\right) \left[\left(\frac{E_0}{E}\right)^{\frac{1}{2}} + 1\right],$$

$$|(k_0^2 - k^2)^2| |G_{1,0}| \le \left| \frac{E}{E_0} - 3 \right| + 2\left(\frac{E_0}{E}\right)^{\frac{1}{2}} + k_0 a \left(1 - \frac{E}{E_0}\right) \left[\left(\frac{E_0}{E}\right)^{\frac{1}{2}} + 1\right].$$

$$\dots (7.1)$$

Column 4 of Table 2 gives maximum possible values of the cross-section obtained by using (7.1) with $E_0 = 10$ MeV.

The cross-sections for Bremsstrahlung on the central exchange force model thus come out very small in the energy range considered; in n-p collisions there would be about 10,000 elastic scattering processes for each such inelastic process. The relative probability for a given direction of the proton has also been investigated and found to be of the same order of magnitude. It thus appears that it would not be possible to detect and measure such radiative collisions with experimental techniques at present available. (In view of the smallness of the cross-sections it would be pedantic to discuss here the question of angular distribution of the particles and photons.) For much higher energies the cross-section for Bremsstrahlung would increase appreciably (at least on this model), and might be capable of measurement. The model used in this paper would, however, be inadequate for treating the problem at high energies with any exactness.

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Resonance Transfer of Electronic Energy in Organic Crystals

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ABSTRACT. The resonance transfer of energy in crystals of organic compounds when excited by visible or ultra-violet light has been examined by measuring the fluorescence of the systems naphthalene-anthracene, anthracene-naphthacene, naphthacene-pentacene, anthracene-acridine, anthracene-phenazine, and anthracene-di- and hexabromobenzenes. The conditions for "exciton" trapping and the relations of resonance transfer to fluorescence quenching are discussed.

§ 1. INTRODUCTION

The transfer of excitation energy by resonance from molecule to molecule in organic crystals is most strikingly shown by the anthracene–naphthacene system (Bowen 1945, Bowen and Mikiewicz 1947). Very small quantities of naphthacene in solid solution in anthracene change the fluorescence from blue to green, the excitation energy travelling by exchange until it is trapped at a naphthacene molecule. This effect disappears when the crystals are dissolved in benzene. The resonance exchange is doubtless assisted by the fact that the flat molecules of anthracene lie nearly parallel in the crystal (Robertson 1932); in the solid solutions the naphthacene molecules are again parallel to them.

For the unambiguous demonstration of the phenomenon it is necessary to use systems where the extinction coefficients show (a) that the exciting light is absorbed by the major constituent, and (b) that the fluorescence of the major constituent is not reduced through secondary absorption by the added substance. For "exciton" trapping to occur the added substance should have a possible transition between energy states associated with a lower energy quantum than a similar transition in the major substance, i.e., should absorb at somewhat longer wavelengths. This implies that the fluorescence band of the latter will almost coincide with the absorption band of the former, but condition (b) will hold if the added substance acts at sufficiently small concentrations. Extinction coefficient measurements are usually wanting for the crystalline state. The crystals are optically highly anisotropic. From the results of Kortum and Finckh (1942) on anthracene, however, it appears that there is little difference between the averaged values for crystals and solutions, except for a shift of about 200 A. of the band to the red in the case of crystals. Solution values have therefore been used after slight correction.

A very high degree of purity is necessary in this work, and the materials used were subjected to careful purification and checked by absorption or fluorescence examination. Mixtures were prepared by weighing the components into a small tube, evacuating, and fusing together. The crystals were ground up and spread in a thin layer on the flat outer side of the inner part of a specially designed metal. Dewar vessel with a silica window for excitation and observation. The fluorescence was excited by a concentrated beam from a small high-pressure mercury arc with filters, and measured through other filters by a photo-electron multiplier unit.

The excitation energy in the crystal may undergo a variety of processes, which may be formally represented by the following scheme, in which the k's are velocity constants, the square brackets indicate concentrations and A^* , $B^* =$ molecules of A, B with excitation energy.

Process	Relative Rate	Description of Process
$A + h\nu = A*$	1	Excitation by light.
$A^* = A + h\nu_1$	$k_1[A^*]$	Fluorescence of major constituent.
$A^* = A$	$k_1 k_2 [A^*]$	Self-quenching of major constituent.
$A^*+A=A+A^*$		Exciton transfer.
$A^*+B = B^*+A$	$k_1k_3[A^*][B]$	Exciton transfer to added substance.
$B^* = B + h_{\nu_2}$	$k_4[B^*]$	Fluorescence of added substance.
$B^* = B$	$k_4 k_5 [B^*]$	
$B^*+B=B+B$	$k_4 k_6 [B^*][B]$	Self-quenching of added substance.
$A^*+B=B+A$	$k_1k_7[A^*][B]$	Quenching by added substance.

The quantum efficiencies of fluorescence are then for A:

$$1/\{1+k_2+k_3[B]+k_7[B]\};$$

and for B:

$$k_3[B]/\{1+k_2+k_3[B]+k_7[B]\}\{1+k_5+k_6[B]\}.$$

§ 2. RESULTS

The following systems were examined and results are shown graphically in Figure 1. Ordinates are fluorescence efficiencies (quantum yields) and abscissae the concentrations of the minor constituent expressed logarithmically (e.g. 7 indicates 10⁻⁷ gm/gm.) except in the case of the anthracene-bromobenzene systems, where they are given as gm. per cent. The values of molar extinction.

coefficients ϵ given below for comparison relate to solutions of the hydrocarbons with a slight correction for band shift in the solid substances.

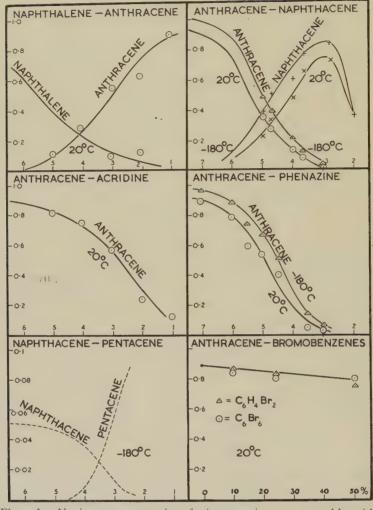


Figure 1. Abscissae: concentration of minor constituent expressed logarithmically (for anthracene-bromobenzene, expressed as a percentage).

Ordinates: fluorescence efficiencies.

Naphthalene with anthracene

Exciting light: 2900-3200 A., filtered by solutions of nickel, cobalt, and copper sulphates.

Absorption: naphthalene 2500–3200 A., $\log \epsilon = 3.5$ at 3000.

anthracene 3200–4100 A., $\log \epsilon = 2.4$ at 3000, and 3.5 at 3650.

Fluorescence: naphthalene 3130-3720 A., estimated by amount of fluorescence cut off by an Ilford 805 filter.

anthracene 4020-5020 A., estimated from total fluorescence less that removed by an Ilford 805 filter.

Crystalline naphthalene has an efficiency of about 0.7 at ordinary temperature, but in the anthracene solid solutions the anthracene fluorescence rises to an

efficiency of 0.9, equal to that of pure anthracene, at a concentration of 10%. At -180° c. the efficience are 0.95 and 1.0 respectively; $k_2 = 0.3$, $k_3 = 5 \times 10^4$ at 20° c., $k_2 = 0.05$, $k_3 = 1.3 \times 10^4$ at -180° c. The other constants are zero.

Anthracene

with naphthacene

Exciting light:

3650 A., filtered by Chance's glass OX 1.

Absorption: anthracene 3200-4100 A., $\log \epsilon = 3.5 \text{ at } 3650.$

naphthacene 3600-5000 A., $\log \epsilon = 2.4$ at 3650, and 4.0 at 4900.

Fluorescence: anthracene 4020-5020 A., estimated through Ilford filter 601.

naphthacene 4900–5750 A., estimated through Ilford filter 404.

The falling off of the naphthacene fluorescence at concentrations above about 0.1% is attributed to self-quenching effects. The limit of anthracenenaphthacene solid solution formation is unknown, but appears to be much greater than 0.1%, so that it cannot be ascribed to the separation of a different solid phase. $k_2 = 0.1, k_3 = 2 \times 10^5, k_6 = 2.5 \times 10^2 \text{ at } 20^\circ \text{ c.}, k_2 = 0, k_3 = 6 \times 10^4, k_6 = 10^2 \text{ at } -180^\circ \text{ c.};$ the other constants are zero.

Anthracene



with acridine



Exciting light:

3650 A.

anthracene Absorption:

3200–4100 A., $\log \epsilon = 3.5$ at 3650.

acridine

 $3000-4300 \text{ A.}, \log \epsilon = 3.6 \text{ at } 3650.$

Fluorescence: anthracene 4020-5020 A.; acridine feeble.

Since the solid solutions containing acridine show practically only anthracene fluorescence the acridine traps and quenches the exciton. $k_2 = 0.1$, $k_7 = 5 \times 10^2$ at 20° c.; the other constants are zero.

Anthracene



with phenazine



Exciting light:

3650 A.

Absorption:

 $3200-4100 \text{ A.}, \log \epsilon = 3.5 \text{ at } 3650.$ anthracene

phenazine

3100-5000 A., $\log \epsilon = 4.0$ at 3650.

Fluorescence: anthracene 4020-5020 A.; phenazine none.

As acridine, phenazine acts as an exciton quencher. $k_2 = 0.1$, $k_7 = 7 \times 10^4$ at 20° c., $k_2 = 0$, $k_7 = 3 \times 10^4$ at -180° c.; the other constants are zero.

The naphthalene-quinolene system is closely similar to this one except that its bands lie at shorter wavelengths.

Naphthacene



with pentacene



Exciting light:

4358 A., filtered by solutions of cuprammonium sulphate and sodium nitrite.

Absorption:

naphthacene 3600–5100 A., $\log \epsilon = 3.5$ at 4358.

4300–6100 A., $\log \epsilon = 2.6$ at 4358 and 4.3 at 6000. pentacene

Fluorescence: naphthacene 5000-5900 A.; pentacene beyond 6000.

Owing to the feeble fluorescence of this system observations could be made only at liquid air temperatures, and even here is was possible only to make rough visual estimations. The absolute values of the fluorescence efficiencies given are very rough approximations: $k_2 = 2 \times 10^2$, $k_3 = 10^6$, $k_5 = 3 \times 10^2$ approx. at -180° C.

Anthracene with p-dibromobenzene and hexabromobenzene.

Exciting light 3650 A.

Though it forms solid solutions with anthracene up to 30% concentration, p-dibromobenzene exerts little quenching effect. Hexabromobenzene behaves similarly. These substances have absorption bands at shorter wavelengths than 3650 A. and appear unable to act as exciton traps, though they act as quenchers for anthracene fluorescence in liquid solutions (Bowen and Norton 1939). In the latter state van der Waals associations of anthracene molecules with bromocompounds appear to be responsible for the quenching (Bowen, Barnes and Holliday 1947).

In addition to the above systems the three-component system anthracene with small quantities of both naphthacene and phenazine was examined. The phenazine diminishes the observed fluorescence coming from both the anthracene and the naphthacene. The two-component system constants given above were found to reproduce the fluorescences observed through Ilford filters 601 and 404 (blue anthracene and green naphthacene emissions) within the limits of error. The agreement between observed and calculated results in all the above instances is only approximate, due to the inevitable inaccuracies of fluorescence measurements from crystals. Large errors occur through variations of light diffusion losses in different preparations. The solid solutions also are far from uniform in composition. When a solid solution of naphthacene in anthracene is prepared, for example, either by fusion or by crystallization from a solvent, the first crystals deposited have a higher naphthacene concentration than the liquid, and as deposition proceeds a series of solid solutions of different compositions are formed successively. The only way out of this difficulty would be to prepare specimens by crystallizing a small fraction only from a liquid and to find its composition by subsequent analysis. This would require large quantities of highly purified materials which were beyond our resources.

§3. DISCUSSION

A quantity of great interest in relation to these systems is the "life" of an exciton process. The mean lives of anthracene fluorescence in the solid and dissolved states are not accurately known. Wood (1921) found a value of about 10-5 sec. for crystalline anthracene, but recent unpublished work indicates that it is really very much smaller. The average life for dissolved anthracene, estimated by the polarization method in glycerol, appears to be 10^{-7} sec., but this is probably too long because the "micro" viscosity of the solvent may be less than the ordinary viscosity. The absorption band areas $\int \epsilon d\omega$ (Lewis and Kasha 1945) give about 10⁻⁸ sec. for both solid and liquid anthracene, assuming the accuracy of the curves of Kortum and Finckh (1942). The exciton movement in the crystal does not seem to cause any great lengthening of the period between absorption and radiation. The question then arises, what terminates the resonance transfer process in the absence of any added trapping agent? There are two possibilities: radiation may occur from molecules which are "displaced" in the crystal, or at the surfaces of "mosaic structure", or the removal of excess vibrational energy from the excited molecule may stop transfer. Figure 2 shows potential energy curves for a diatomic molecule.

Absorption is represented by the vertical line BK and fluorescence by GM. The time for passage from K to G is about 10^{-12} sec. It might be assumed that exciton transfer continues while the energy available is represented by point K,

but that when a molecule falls to G it has insufficient energy for an energy exchange chain.

A further matter of interest is the alternative of radiation or quenching in these crystals. Quenching is undoubtedly favoured by polarizability effects (Bowen 1947). The series of solids anthracene, naphthacene and pentacene have fluorescent efficiencies at 20° c. of about 0·9, 0·002, and 0 respectively, probably due to increasing polarizability of the molecules. When embedded in an anthracene crystal naphthacene and pentacene molecules fluoresce with much higher efficiencies. If two polarizable molecules approach closely, their potential-energy curves (see Figure 2) become shifted and less well defined, especially in the region

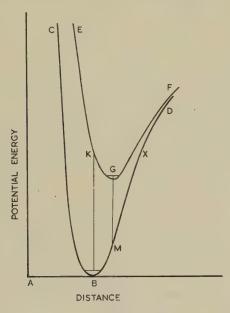


Figure 2.

marked X. Radiationless transition to the ground state is then possible, the excitation energy passing into vibrational energies of the two molecules. Resonance transfer of energy, however, occurs at larger distances, where polarizability has less effect, but where there is sufficient electronic interaction present. Both processes may be visualized as initiated by the transfer of an electron from an unexcited molecule to the vacated orbital of an excited one with transfer of the excited electron in the reverse direction. If the transfers are simultaneous the process gives rise to the exciton, but any check between them may lead to quenching. How these two effects depend on the relative orientations of molecules to each other with ensuing directional effects in the crystal is a matter about which we know little at present.

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Further Experiments with an Adjustable Geiger-Müller Counter

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ABSTRACT. An adjustable Geiger-Müller counter and special electronic circuits have been used to study the effect of several counter variables on the occurrence of multiple pulses. The results show that the plateau characteristics combine the effects of an increase in efficiency and an increase in the probability of a multiple pulse as the operating potential is raised. It was found that the probability of occurrence of multiple pulses does not depend simply upon the charge per pulse, but that it depends also upon the anode diameter and the total pressure of the filling.

Curves have been drawn showing the charge per pulse as a function of the operating potential. A change of slope occurs in these curves when the charge per pulse is approxi-

mately equal to the charge on the active portion of the anode.

The counter was used as an ionization chamber at operating potentials below the Geiger region. It was found that as the potential is raised above the threshold of the proportional region the ionization current varies with potential as $\log I \propto V$ while at higher potentials the relation is adequately expressed by $\log \log I \propto V$. Near the Geiger region a sharp break occurs in the $\log \log \operatorname{curve}$, which is taken to indicate that the discharge begins to spread at this stage.

§ 1. INTRODUCTION

In a previous paper (Chaudhri and Fenton 1948, subsequently referred to as I) it was shown that with a given cathode and filling the length and slope of the plateau depend strongly on the anode diameter. The present paper is a report of work primarily intended to extend the investigations to include the effect of pressure on the plateau characteristics.

Previous workers (see for example Korff and Present 1944, Curran and Rae 1947) have attributed the slope of the plateau to spurious pulses and to an increase in the effective anode length as the operating potential is raised. It is convenient to divide the spurious pulses into two classes: (a) those pulses which occur as a result of previous pulses and are separated from them by time intervals of the order of several hundred microseconds; (b) pulses which are not the result of the entry of any ionizing particle into the effective volume of the counter.

Pulses of type (a) may be distinguished by their non random distribution while pulses of type (b) can be distinguished if the rate at which they occur depends on the counter variables. In particular, to affect the plateau slope the rate must vary with operating potential. In view of the observation that the plateaux corrected for spurious pulses of type (a) are the same within experimental fluctuations over the range of pressures and anodes used, we believe that very few pulses of type (b) occur in our counter.

To study the contribution of spurious pulses of type (a) to the plateau characteristics an interval discriminator circuit was used during the measurements. During the course of the work the charge per pulse was measured over the range of operating potentials for each anode and pressure. The counter was also used as an ionization chamber and the results provide interesting information about the threshold of the Geiger region.

For convenience we give below a list of the symbols and definitions used in the report.

 $V_{\rm s}$ threshold of the Geiger region.

M number of square waves per second produced by the multivibrator.

C number of coincidences per second.

R counting rate in counts/second excluding spurious pulses of type (a).

S number of spurious pulses of type (a) per second.

G total counting rate in counts per second.

P measured probability that any pulse will produce as purious pulse of type (a). P = S/G.

 $t_{\rm d}$ dead time, i.e. the time which elapses after the occurrence of a pulse before another Geiger discharge can occur.

q charge per pulse.

§ 2. APPARATUS AND EXPERIMENTAL METHODS

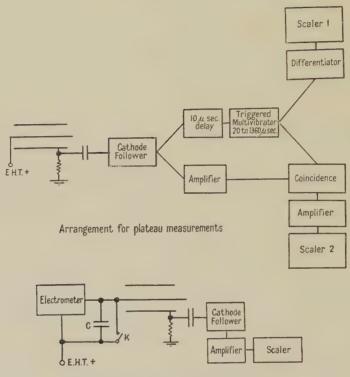
The adjustable counter described previously (I) was used during the present observations. The counter was set so that the central 5 cm. length of the anode was used, and the filling was 90% of spectroscopically pure argon plus 10% of alcohol. The tungsten anodes used were of 0.05, 0.07, 0.1, 0.15, and 0.20 mm. diameter. The gas pressure could be changed without pumping and refilling (a process which has proved to be not reproducible with our set-up) by adjusting the level of mercury in a 1-litre flask attached to the system. In view of the experiments reported by Korff (1944) no trouble was to be expected due to the small amounts of mercury vapour thus introduced into the counter. Throughout the work to be described the pressure could be set at any value from 7.5 to 19 cm. of mercury, the pressure being read from a U-tube manometer. Relatively low counting rates (of the order of 1,000 per minute) were used because earlier results had shown that high counting rates alter the background (I).

To find the contribution of spurious counts to the plateau characteristics the circuits shown in Figure 1 were used with the triggered multivibrator set to give waves of $1,000\,\mu\text{sec.}$ duration, thus dividing the Geiger counts into two groups: group 1, recorded by scaler 1, counts occurring at any time greater than $1,000\,\mu\text{sec.}$ after the previous count, group 2 (scaler 2), those occurring less than $1,000\,\mu\text{sec.}$ after the previous count.

A small correction was made for the number of random counts in group 2. Because of the dead time of the counter during which no pulses, random or otherwise, can occur, the effective time interval used for the calculation of the number of random pulses likely to occur is $1,000\,\mu \rm sec$. minus the dead time. The dead times were therefore measured, for each operating potential during the plateau measurements, by decreasing the length of the square wave until no coincidences occurred.

It was shown that all spurious counts occur within 1,000 μ sec. of the previous pulse by measuring the rate at which spurious counts occurred for a series of values of the multivibrator interval at constant operating voltage. The spurious rate increased rapidly with multivibrator interval at first but ultimately became more constant. This measurement was made at points near the beginning, the middle, and the end of the plateaux for each anode using a pressure of 12 cm. Hg. The time value at which the rate ceases to increase with interval was always found to be less than 1,000 μ sec. A check was made at other pressures by increasing the interval from 1,000 to 1,360 μ sec. and as this gave no increase in S it was concluded that all the spurious counts occur within the 1,000 μ sec. interval.

For the charge measurements a type 954 acorn valve was used in an electrometer circuit attached to the anode of the counter as shown in Figure 1. In practice the opening of the key K was synchronized with the closing of the scaler counting switch, and the number of counts necessary to alter the potential of the grid of the electrometer valve by 0.5 volts was registered. Hence the average charge per pulse can be calculated, using the measured capacity of the system.



Arrangement for pulse size measurements

Figure 1.

When the counter was used as an ionization chamber the electrometer was employed to indicate the collection of a predetermined charge in a measured time. By altering the capacity C it was possible to measure over a large range of ionization currents without having to measure either very short or very long time intervals. The currents measured ranged from about 2×10^{-13} to 10^{-8} amp. when the gammaray source was placed close to the counter. An additional factor of about 100 was obtained in two stages by moving the source away from the counter, so that in effect the measurements covered the current range from about 2×10^{-13} to 10^{-6} amp.

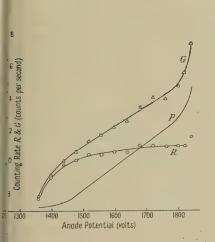
§ 3. RESULTS

3.1. Plateau Characteristics

The curves obtained have the general form shown in Figure 2. The corrected plateaux corresponding to the various pressures and anode diameters give the shape of the plateaux that would be obtained if there were no multiple pulses. Graphs of these lie close together when plotted with the same counting rate and

overvoltage coordinates. As there are no observable trends of variation with pressure or anode diameter it appears that the shape of the corrected plateau is, from the practical viewpoint, independent of these variables over the range covered by the present experiments. Eventually, as the potential is raised, the corrected plateau breaks off due to sprays of multiple pulses lasting more than 1,000 µsec.

The curves of P plotted against operating potential vary considerably with



rigure 2. Typical plateau analysis.

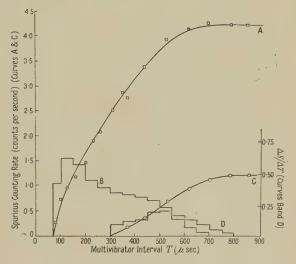


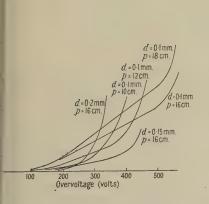
Figure 4.

Counter data: Anode diameter 0.07 mm.

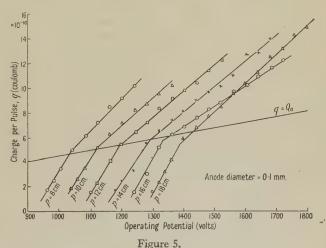
Total pressure 12 cm.

Operating Potential: A and B 1,440 v.

C and D 1,240 v.



3. Variation of P with overvoltage for various anode diameters (d) and total pressures (p).



pressure and with anode diameter (Figure 3). For purposes of comparison it is convenient to plot, as a function of the potential, the probability that a multiple count occurs, instead of the spurious counting rate. The results show that *P* increases rapidly at overvoltages corresponding to the upper ends of the Geiger plateaux; the overvoltage at which this rapid increase begins increases as the

anode diameter is reduced from 0.2 mm., passes through a maximum at an anode diameter of about 0.1 mm. and then decreases. The slope of the straight portion of P curves increases the anode diameter is reduced.

3.2. Spurious Count Distribution

The curves obtained by plotting the spurious counting rate against multivibrator interval show that the spurious counts begin to occur immediately after the dead time (Figure 4, curves A and C). As measured above, $t_{\rm d}$ is the time after a pulse during which the counter is unable to give a pulse as great as the minimum detectable size. By observing the pulses on a triggered cathode-ray oscillograph it was shown that this minimum size is reached after about $1\cdot 1$ of the true dead time and that pulses smaller than this minimum detectable size also occur more frequently than the random rate.

The distribution in time of the spurious counts was obtained by taking a histogram of the curves of S plotted against multivibrator interval. Except at high overvoltages the maxima of these histograms occur at a time approximately equal to that required for the space charge to cross the counter, assuming an ionic mobility intermediate between those given in the International Critical Tables for argon ($k=1.66\,\mathrm{cm/sec}$. per v/cm.) and alcohol ($k=0.48\,\mathrm{cm/sec}$. per v/cm.). Figure 4, curve B, is for a high overvoltage. At overvoltages near the middle of the plateau and below the histograms are nearly symmetrical (Figure 4, curve D).

3.3. Pulse Size Measurements

Figure 5 shows the average charge per pulse q plotted against the operating voltage for a series of pressures using the $0\cdot1$ -mm. diameter anode. The line $q=Q_0$ gives the charge on the active length (5 cm.) of the counter wire. With anodes of diameter $0\cdot05$, $0\cdot07$ and $0\cdot1$ mm. and at pressures ranging from 8 cm. to 18 cm. Hg a sharp break occurs in the curves at about $q=Q_0$ while the ratio of the slopes of the lines on either side of the break ranges from $0\cdot4$ to $0\cdot67$. For larger anodes $(0\cdot15$ and $0\cdot2$ mm. diameter) and at the higher pressures the break occurs for $q< Q_0$ and the slope ratio increases.

In Figure 6 the charge obtained at a total pressure of 10 cm. Hg is plotted against overvoltage for four different anode wires. The curves show that the charge at a

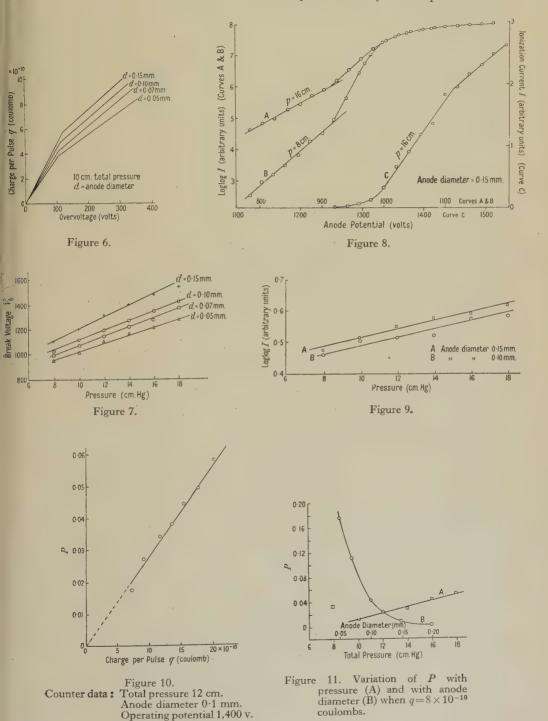
given overvoltage increases slowly with increasing anode diameter.

The break voltage also increases with increasing wire diameter. The starting voltage, from which these overvoltages are obtained, is defined as the voltage at which the extrapolated $q \sim V$ curve shows q = 0. Figure 7 shows that the break voltage increases linearly with pressure for all anodes where the break is clearly defined.

3.4. Measurement of Ionization Current

The counter was used as an ionization chamber, connected as shown in Figure 1. As the potential is raised above the proportional starting voltage $V_{\rm p}$ the logarithm of the ionization current I is proportional to the potential at first; then at higher potentials $\log \log I$ becomes proportional to potential as shown in Figure 8, curves A and B. Sharp breaks occur in the $\log \log$ curves and when these are matched, as shown in the figure, the curves for different gas pressures converge as the potential is raised. Figure 8, curve C shows I plotted against potential for the region above the break for 16 cm. pressure. This curve may be

compared with the charge per pulse curves of Figure 5. Figure 8, curve C shows that the value of V_s as defined in §3.3 is about 50 v. above the potential given by the break in the log log curve. Figure 9 shows that the value of log log I at the break in the log log curves depends linearly on the pressure.



3.5. The Dependence of P on q

The probability P of the occurrence of spurious pulses and the charge per pulse q were obtained as functions of the anode length, and from the resulting straight line relationships the relation between P and q was obtained. Figure 10 shows the linear dependence of P on q for a 0·1 mm. anode, 10% alcohol, and 12 cm. Hg total pressure, at a fixed operating potential of $1,400\,\mathrm{v}$. This method of varying q has the advantage that as the operating potential is held constant the discharge mechanism does not alter, the charge increasing with anode length simply because the discharge has further to spread. The possibility that the variation of counting rate with anode length may have some effect on the value of P was removed by using a fixed anode length and altering the position of the gamma-ray source to cover the range of counting rates obtained during the experiment in which the anode length was varied. P was found to be independent of R over this range.

In order to find the dependence of P on the anode diameter and the pressure of the filling a fixed value of q was chosen and the corresponding values of P were taken from the Pvs ($V-V_s$) curves, examples of which are shown in Figure 3. The results are shown in Figure 11 where the values of P corresponding to $q=8\times 10^{-10}$ coulombs are plotted against pressure (curve A) and anode diameter (curve B). This value of q was chosen because, with the exception of the value at 8 cm. total pressure the corresponding values of P lie on the early portions of the Pvs ($V-V_s$) curves, in the region where the majority of the multiple pulses contain only two individual pulses. The rapid increase of P corresponding to the upper limit of the plateau is associated with multiple pulses of multiplicity greater than two.

§ 4. DISCUSSION

The corrected plateaux of which an example is given in Figure 2 do not flatten to any extent until the operating potential is appreciably above the threshold. Further, as can be seen with a cathode-ray oscillograph, the pulses are of approximately equal size before the apparatus begins to register counts (minimum detectable pulse size = $1 \cdot 2$ v.). It has also been shown by varying the amplifier gain that the increase in the corrected counting rate with operating potential is not due to small pulses being brought within range of the apparatus. Part of the increase may be due to an increase in the effective length as mentioned in §1, but because of the method of shielding the anode used in our counter we do not think that end effects can account entirely for the observed increase . On the other hand, plateaux of this form are predicted by Narwijn (1943) and Wilkinson * who obtain the probability that the discharge begins to spread as a function of overvoltage.

For one electron set free in the counter by the ionizing agency this probability is rather low (0.6) at an overvoltage of about 50 v. (i.e. when counts are first registered) and increases with overvoltage to about unity at 200 v. above the threshold, corresponding to a fairly large slope in the corrected plateau. At a fixed overvoltage the probability of spreading increases as the specific ionization increases, and at 50 v. overvoltage is practically unity when the number of electrons set free by the ionizing particle exceeds five. A gamma-ray photon can only be detected if it releases an electron which then enters the effective volume of the counter. In our case the gamma rays from radium are filtered by 3 cm. of lead so that most of the primary electrons will have energies of 1 MeV. or over. Depending

^{*} We are indebted to Dr. D. H. Wilkinson, Cavendish Laboratory, Cambridge, for this information prior to its publication.

on its path through the counter, from one to about eight secondaries will be produced by an electron of this energy, so that we should not expect the plateau to flatten until appreciable overvoltages are used. From the practical standpoint the corrected plateau curves show that in a counter such as ours the overvoltage used should be of the order of 200 v. This would apply also when the cathode is treated to reduce spurious pulses to a minimum, or when a paralysis circuit is used to prevent their being counted.

It was reported earlier (I) that there is an optimum anode diameter corresponding to a given filling and cathode for which the best Geiger plateau is obtained. This observation is explained in terms of the way in which the spurious counting rate curves vary with anode diameter and the way in which they combine with the corrected plateaux to give the Geiger plateaux. It should also be pointed out that the sum of the corrected plateau and the spurious counting rate curve does not always yield a curve with a really straight portion. This explains the deviation of points sometimes observed from the straight lines usually drawn for the Geiger plateaux, even when a large number of counts are taken in order to reduce the standard deviation.

The sharp breaks in curves A and B of Figure 8 are interpreted as marking the stage at which the discharge begins to spread along the anode. This view is supported by observations with a cathode-ray oscillograph in the neighbourhood of the break. A few volts above the potential corresponding to the break there is a distribution of pulse sizes. The maximum pulse size observed at a given operating potential is halved by halving the effective length of the counter, showing that at quite low overvoltages the discharge can spread to the full length (10 cm.). As the potential is raised the number of pulses reaching the corresponding maximum size increases until at about 20 volts overvoltage all the pulses appear to be of the same size. The starting potential for the Geiger region is generally defined (Korff 1944) as the potential at which all the pulses are of equal size. While this definition is usually adequate for the practical use of counters it simply indicates the potential at which the discharge spreads to the full length of the counter, and because of the statistical nature of the spreading mechanism (Alder et al. 1947, Wilkinson, unpublished) its value depends on the counter length. However, when the discharge mechanism is being investigated the potential at which spreading begins is often of importance and this may be determined quite simply by the method described in this paper.

The observed dependence of the probability of occurrence of spurious counts on the charge per pulse is consistent with the view expressed by Korff (1944) that multiple pulses are due to statistical breakdown in the quenching mechanism which occurs when the positive ions reach the cathode. However, P does not depend only on the number of ions reaching the cathode but, as shown in Figure 11, depends also on the anode diameter and the pressure. These results suggest that the ions which arrive at the cathode are not all of the same type, and that the production of the ions which are more likely to produce spurious pulses is favoured by the use of high pressures and small anode wires. The effect may be due to the increase in the field near the anode when smaller anodes or higher pressures are used. Calculation of the fields at the anode surfaces using the operating potentials corresponding to the points given in Figure 11 yields values of the field strength ranging from 37,000 v/cm. for the 0.2 mm. anode to 110,000 v/cm. for the 0.05 mm. anode. For the 0·1 mm. anode it ranges from 49,000 v/cm. at 8 cm. pressure to 64,000 v/cm. at 18 cm. pressure.

The spurious count distribution curves (e.g. Figure 4) together with the observations with a triggered cathode-ray oscillograph show that some spurious pulses occur as soon as the end of the dead time is reached and that the pulses are distributed over a fairly wide range of times. These curves also provide evidence that the ions formed in the discharge are not all of the same type. The distributions obtained at low voltages are symmetrical, as would be expected if the space charge is regarded as a group of ions moving with a Maxwellian velocity distribution upon which one drift velocity (due to the electric field) is imposed. This applies in the outer part of the counter where the field varies slowly so that focusing is negligible and ions of the one type have approximately constant drift velocity. At high voltages the distribution curves are characterized by a sharp rise to the maximum followed by a very gradual fall. Such a distribution would be given if the space charge contained multiply, as well as singly ionized atoms; the higher drift velocity imposed on the multiply ionized group would give the early maximum and the subsequent arrival of the singly ionized group would explain the very gradual fall. This view is supported by the fact that the asymmetry sets in at points lower on the plateau for the smaller anodes, as here the field strength at the wire is greater. The continuous electron transfer between singly ionized argon atoms and alcohol molecules which, according to Korff (1944), explains the quenching action, does not affect the argument. Such a transfer affects the position of the maximum because of the difference in the mobilities of the ions, but it could not produce the observed asymmetry as the exchange is complete before the ion sheath reaches the cathode.

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The Steady Non-Uniform State for a Liquid

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MS. received 12th August 1948

ABSTRACT. The Smoluchowski equation for the distribution of the relative coordinates of a representative pair of molecules in a liquid is formulated in such a way that the effect of non-uniform velocity or temperature is taken into account. The equation is reduced to an ordinary linear differential equation of the second order. One of the two constants of integration is readily determined whereas the determination of the other constant may lead to inconsistencies. The molecules are assumed to interact with the average potential that is appropriate to thermal equilibrium. If it is assumed that this potential becomes infinite of the first order at distance zero then the problem of viscous flow and the problem of thermal conduction are uniquely soluble. Approximate evaluation of the transport coefficients shows the right kind of temperature effect. The result is in accordance with the previous treatment by means of the cell model.

§ 1. INTRODUCTION

In a previous paper (1947) referred to as I the author analysed the transport phenomena in liquids by means of extremely simplified assumptions on the liquid state. The "cell model" was employed and the Smoluchowski equation was used for determining the distribution in coordinates of one representative molecule. The influence of the rate of shear or gradient of temperature on the distribution was taken into account only on the surface but not in the interior of the cell. The calculated distribution functions were infinite at the centre of the cell but yielded finite values for the flow of momentum or energy. The marked difference of the temperature effect on viscosity and thermal conductivity was obtained without any additional assumption and in spite of the complete similarity of mathematical operations which lead to the one and to the other transport coefficient.

The author was unaware of a paper by Auluck and Kothari (1944) in which formulae similar to the author's are derived from the well-known "hole" model as given by Fürth (1941); in addition, numerical values of the right order of magnitude are obtained. In their paper the mechanism and the rate of transfer is explicitly assumed to be markedly different for momentum and energy. The author's result shows at least that assumptions of this kind are unnecessary.

In the meantime Born and Green (1947) published the extension of their general kinetic theory of liquids to transport phenomena and made a preliminary calculation of the viscosity; in their result various approximations are involved and the equilibrium distribution of a pair of molecules in a liquid is replaced by the distribution of a pair of isolated molecules. Since thermal conductivity still awaits detailed treatment, and the introduction of the liquid state distribution may affect the result appreciably, it cannot yet be seen to which conclusions the rigorous theory, as developed by these authors, will lead.

The method as employed in paper I is too crude for the actual calculation of the transport coefficients. In addition, its foundations, that is, the cell model and the application of the Smoluchowski equation, are open to criticism.

The cell model is hardly suitable for a quantitative theory since it is impossible to divide the liquid into cells of fixed size and shape without introducing arbitrary and sometimes inconsistent assumptions. The partial success of this model is due to the fact that fundamentally it is an approach to the specification of the liquid state in terms of the distribution of relative coordinates of two representative molecules.

The Smoluchowski equation is at first sight a legitimate approximation to the equation which has been shown by Kirkwood (1946) to be adequate and it is preferable from the point of view of mathematical simplicity. Its application in paper I resulted, however, in distributions which are infinite at one point.

In the present paper an attempt is made to clear the ground for the calculation of transport coefficients by employing the pair distribution instead of the cell model and by admitting only solutions of the Smoluchowski equation which, when interpreted as probability distributions, are in agreement with the physical conditions.

§ 2. THE MODEL OF THE LIQUID STATE

In this paper the liquid state is described in terms of the relative coordinates of two representative molecules. The probability distribution of the relative coordinates of the two molecules is, in the case of monatomic liquids, a probability distribution of the distance r. The assumption is made that the two molecules interact with a force equal to the negative gradient of an average potential $\Phi(r)$ which itself is derived from the equilibrium distribution.

The probability density in equilibrium is zero at small distances, has one strong and possibly several weak maxima and tends to a constant value at large distance. It can be derived from experimental x-ray interference patterns or calculated from the intermolecular forces according to the theory of Kirkwood (1935) or Green (1947).

The average potential Φ which is essential for the model under consideration is defined by writing the equilibrium distribution $g_0(r)$ as

$$g_0(r) = (1/V)\exp(-\Phi/kT).$$
 (1)

 Φ depends according to this definition explicitly on the temperature, but little is known of the amount of this dependence. In equilibrium only the minima of potential are densely occupied; in non-equilibrium distributions all ranges of the potential curve may be of importance. For large distances Φ is zero. Where the potential is markedly positive it is not likely to depend very much on the temperature. Near the main minimum at about one molecular diameter distance, the potential varies with temperature so that the minimum becomes flatter when temperature decreases; this variation is an expression of the fact that the molecules have not the tendency to crowd together at the distance of the minimum. At small distances the potential is likely to approach the repulsion potential of a pair of isolated molecules. If overlapping of the electronic clouds is almost complete—the corresponding small distances are practically never reached—the potential becomes infinite of the first order owing to the Coulomb repulsion of the nuclei.

For the model under consideration the Smoluchowski equation has to be modified in order to account for the non-uniform velocity or temperature independently of the boundary conditions.

§ 3. THE DIFFERENTIAL EQUATIONS

If temperature and velocity are uniform, the distribution, g, of relative coordinates is determined by the Smoluchowski equation

$$\partial g/\partial t = \operatorname{div}[\operatorname{grad}(kTg/\beta m) + (g\operatorname{grad}\Phi/\beta m)], \qquad \dots (2)$$

where β is the "friction constant" having the dimension time⁻¹, $-\operatorname{grad} \Phi/\beta m$ is the mean displacement, $kT/\beta m$ is the mean square displacement per time unit; the expression in the bracket is equal to the negative flow vector \mathbf{j} . In thermal equilibrium $g = g_0$, $\mathbf{j} = 0$.

For a steady non-uniform state let $g = g_0(1+w)$. For the specification of viscous flow let the velocity \mathbf{c} depend in an arbitrary way upon the coordinates subject to the condition div $\mathbf{c} = 0$; \mathbf{c} is added to the mean displacement. Neglecting terms of the magnitude $\mathbf{c} \cdot w$, the flow is then given by

$$\mathbf{j} = g_0[\mathbf{c} - (kT/\beta m) \operatorname{grad} w]$$
(3 a)

and w is determined by

$$\nabla^2 w - (\operatorname{grad} \Psi, \operatorname{grad} w) = -(\beta m/kT)(\mathbf{c}, \operatorname{grad} \Psi), \dots (4a)$$

where $\Psi = \Phi/kT$ subject to the boundary condition

$$\operatorname{grad} w = 0 \quad (r = \infty) \qquad \dots (5 a)$$

so that in infinity the flow is equal to g_0 . **c**.

For specifying thermal conduction let T be an arbitrary function of the coordinates subject to the condition $\nabla^2 T = 0$. Neglecting terms of the magnitude w grad T, grad T etc., the flow is given by

$$\mathbf{j} = -(k/\beta m)g_0[T_0 \operatorname{grad} w + (1 + \Psi) \operatorname{grad} T], \qquad \dots (3b)$$

where T_0 is the temperature at the origin and w is determined by

$$\nabla^2 w - (\operatorname{grad} \Psi, \operatorname{grad} w) = (\Psi/T_0)(\operatorname{grad} \Psi, \operatorname{grad} T), \dots (4b)$$

subject to the boundary condition

$$T_0 \operatorname{grad} w + \operatorname{grad} T = 0$$
 (5 b)

so that the flow is zero at infinity.

For the purpose of calculating viscosity let the flow be laminar with a rate of shear equal to $\frac{1}{2}a$ and the velocity be distributed according to $c_x = c_z = 0$; $c_y = ax$. Then the right hand side of (4a) is $-\alpha \Psi'r \sin^2\theta \sin\phi \cos\phi$; $\alpha = a\beta m/kT$. Let w have the form $w = u(r)\sin^2\theta \sin\phi \cos\phi$. The function w changes sign at $\phi = 0$, $\pi/2$, π , $3\pi/2$. If one molecule is placed arbitrarily at the centre the probability that the other will be in one pair of quadrants, say 1 and 3, is greater than that it will be in the other quadrants 2 and 4. This means that in the flowing liquid the distribution of molecules is anisotropic. The function u is determined by

$$u'' + [(2/r) - \Psi']u' - (6u/r^2) = -\alpha \Psi' r,$$
(6 a)

with the boundary condition

$$du/dr=0$$
; $u/r=0$ $(r=\infty)$ $(7a)$

For the purpose of calculating thermal conductivity let the temperature be distributed according to $T = T_0(1+bz)$ so that the gradient is constant: $\operatorname{grad}_x T = \operatorname{grad}_y T = 0$; $\operatorname{grad}_z T = bT_0$. Then the right-hand side of $(4 \ b)$ is $b \Psi \Psi' \cos \theta$. Let w have the form $w = v(r) \cos \theta$, then v is determined by

$$v'' + \lceil (2/r) - \Psi' \rceil v' - (2v/r^2) = b\Psi\Psi'$$
 (6 b)

with the boundary condition

$$dv/dr = -b$$
; $v/r = -b$ $(r = \infty)$(7b)

The calculation of the transport coefficients is reduced to the integration of the radial differential equations (6 a), (6 b). Which solutions are admissible must be decided by considering how the probability for finding the relative coordinates in a finite volume deviates from the equilibrium distribution. This deviation of probability is proportional to

$$J_a = \int_0^r g_0 u r^2 dr$$
 and $J_b = \int_0^r g_0 v r^2 dr$

respectively. These integrals must be finite for every finite value of the upper limits.

It is known from experiments that laminar flow does not cause any appreciable anisotropy in liquids composed of simple molecules. The integral J_a to which the probability of preferential distribution in an odd quadrant is proportional, gives a measure of anisotropy, and it follows from what has been said that even if the upper limit becomes infinite the integral J_a must remain finite. No restriction of this kind is expected to hold for the integral J_b .

§ 4. SOLUTIONS NEAR THE SINGULAR POINTS

Integration of equations (6a), (6b) near their singular points at the origin and at infinity provides the means for selecting solutions of physical significance.

 Ψ has a pole of the first order at the origin; it will alternatively also be assumed that $\Psi(0)$ is finite. $\Psi' = 0$ if r is sufficiently large.

The two arbitrary constants of integration are denoted by A_1 , A_2 and B_1 , B_2 . Other constants appearing in the solutions are denoted by F and H with suitable suffixes.

The homogeneous equation corresponding to (6a) is

$$u'' + [(2/r) - \Psi']u' - (6u/r^2) = 0.$$
 (8 a)

If the term $-\Psi'u'$ is omitted an equation results which has the solutions $u=r^2$ and $u=1/r^3$.

At large values of r equation (8 a) has accordingly two solutions, one being finite at the origin and of the form

$$u_1 = F_1 r^2 + F_2 / r^3 + 0 (r^{-4}),$$
 (9 a)

the other vanishing at infinity and of the form

$$u_2 = 1/r^3 + 0(r^{-4}).$$
(10 a)

Assuming at first that $\Psi(0)$ is finite, it is seen that at r=0 the expansion of u_1 commences with the second power of r; it can be written as

$$u_1 = r^2 + \frac{1}{3}r^3\Psi'(0) + \dots$$
 (11 a)

The other solution has near the origin the form

$$u_2 = F_3/r^3 + \dots$$
 (12 a)

The general solution of equation (6 a) can be written as

$$u = A_1 u_1 + A_2 u_2 + u_3 \qquad \dots (13 a)$$

where $u_3 = \frac{1}{2}\alpha r^2$,(14 a) is a particular solution.

If the potential has a pole at the origin so that for $r < r_0$ it is equal to $\Psi = C/r$, this does not affect u_3 and the expressions (9 a), (10 a). In the range $0 \le r \le r_0$ the appropriate expressions for u_1 , u_2 are found to be

$$u_1 = u_1^*; u_1^* = 1 + (6r/C) + (12r^2/C^2); u_2 = F_4 u_1^* + F_5 u_2^*; u_2^* = [1 - (6r/C) + (12r^2/C^2)] \exp(C/r)$$
 \tag{15 a}

Equation (6b) is discussed in a similar way. The corresponding homogeneous equation

$$v'' + [(2r/v - \Psi')v' - (2v/r^2) = 0 \qquad \dots (8b)$$

has, for large values of r, solutions of the form

$$v_1 = H_1 r + H_2 / r^2 + 0(r^{-3}),$$
(9 b)

$$v_2 = 1/r^2 + 0(r^{-3}).$$
(10 b)

If $\Psi(0)$ is finite the expansion of v_1 at r=0 can be written

$$v_1 = r + \frac{1}{4}r^2\Psi'(0) + \dots$$
 (11 b)

The other solution has near the origin the form $v_2 = H_3/r^2 + \dots$

The general solution of (6 b) can be written as

$$v = B_1 v_1 + B_2 v_2 + v_3, \qquad \dots (13 b)$$

where the particular solution v_3 is given by

$$v_3(r) = -b \int_0^r \Psi(\xi) \Psi'(\xi) \exp\{-\Psi(\xi)\} \xi^2 [v_2(r)v_1(\xi) - v_1(r)v_2(\xi)] d\xi, \quad \dots (16)$$

and has at large values of r the form

$$v_3 = bH_6r + bH_7/r^2 + 0(r^{-3}).$$
 (14 b)

If the potential has a pole at the origin the appropriate expressions for v_1 , v_2 in the region $0 < r \le r_0$ are found to be

$$v_{1} = v_{1}^{*}; v_{1}^{*} = 1 + (2r/C); v_{2} = H_{4}v_{1}^{*} + H_{5}v_{2}^{*}; v_{2}^{*} = [1 - (2r/C)]\exp(C/r)$$

$$v_{3}^{*} = b\{[1 + (2r/C)][2(r_{0} - r) + C \ln(r/r_{0})]$$

and

+
$$[1 - (2r/C)][2r - C \exp(C/r) \int_{C/r}^{\infty} \exp(-\xi) \xi^{-1} d\xi]$$

is substituted for v_3 . At the origin the function v_2^* and its derivative

$$dv_2^*/dr = -[(C/r^2) + (2/r) - (2/C)] \exp(C/r)$$
(17)

are exponentially infinite and v_3 is infinite of the order $\ln r$.

§ 5. SELECTION OF SIGNIFICANT SOLUTIONS

In determining the constants of integration it is at first assumed that $\Psi(0)$ is finite.

In the problem of viscous flow the first condition (7 a) is applied to (13 a); considering (9 a), (10 a), (14 a) an equation determining A_1 is derived:

$$A_1 F_1 - \frac{1}{2} \alpha = 0. (18 a)$$

The corresponding choice of A_1 complies with the second condition (7 a). The constant A_2 has to be chosen so that the probability J_a is finite for infinite r.

If A_2 is assumed to vanish, J_a becomes infinite owing to the second term in (9 a). If $A_2 \neq 0$, the integral determining J_a is divergent. No solution of (6 a) is admissible.

In the problem of thermal conduction the first condition (7b) is applied to (13b); considering (9b), (10b), (14b) an equation determining B_1 is derived:

$$B_1 H_1 + b H_6 = -b. (18b)$$

The corresponding choice of B_1 complies with the second condition (7b). The integral determining J_b converges independently of any choice of the constant B_2 although the integrand is infinite at the origin if $B_2 \neq 0$. The assumption $B_2 = 0$ is most plausible but not necessary; the distribution and consequently the thermal conductivity remain undetermined.

These difficulties are overcome by letting the potential have a pole at the origin. In the problem of viscous flow A_2 is determined so that r^3u vanishes at infinity:

$$A_1F_2 + A_2 = 0.$$
(19 a)

Whereas u is now exponentially infinite at the origin, the integrand of J_a is finite and the integral is finite for infinite distance. In the problem of thermal conduction the constant B_2 is not determined by considering J_b . The integrand of (25 b) determining the flow of energy contains terms which are proportional to $(r\Psi'-\Psi')g_0v'r^2$. At the origin the expression in the bracket is proportional to 1/r and according to (15 b) and (17) v' is proportional to $1/r^2$ if there is any contribution of v_2^* to v. In order to prevent the flow of energy becoming infinite it is therefore necessary to let

$$B_2 = 0. (19 b)$$

The necessity of specifying the potential near the origin in detail is due to the limit of validity of the Smoluchowski equation. Near the origin the calculated functions cannot be expected to be good approximations; in the problem of viscous flow the correct probability density is likely to be much smaller than g_0u . The contribution of the region near the origin to the flow of momentum or energy is, however, small since the corresponding integrands vanish.

§ 6. APPROXIMATE INTEGRATION

Approximate expressions for the distributions are found by solving differential equations which are distinct from the correct equations by relatively small terms. If $\Psi(0)$ is finite and γ is a constant let

$$f_1(r) = \frac{1}{5}r^2 + \gamma r^{-3} \int_0^r [\exp \Psi(\xi) - 1] \xi^4 d\xi.$$
 (20 a)

This function solves the equation

$$u'' + [(2/r) - \Psi']u' - (6u/r^2) - [3f_1 - (1 - \gamma)r^2](\Psi'u/rf_1) = 0, \quad \dots (21 \ a)$$

which differs from (8a) by the last term only. Transformation of (8a) by means of

$$u = u_0 \exp \frac{1}{2} \Psi, \qquad \dots (22 a)$$

gives
$$u_0'' + [(\Psi'/r) + \frac{1}{2}\Psi'' - \frac{1}{4}\Psi'^2 - (6/r^2)]u_0 = 0.$$
 (23 a)

Substituting (22 a) in (21 a) with $\gamma = 0$ and $\gamma = 1$ yields equations differing from (23 a) by $2\Psi'u_0/r$ and $-3\Psi'u_0/r$ respectively. They are small compared with

the second term of (23 a), particularly if $|\Psi'| > 1/r$ or $\Psi' = 0$. f_1 is therefore an approximation to u_1 and the other solution of (21 a)

$$f_2 = pf_1$$
 $p(r) = -\int_r^{\infty} [\xi f_1(\xi)]^{-2} \exp \Psi(\xi) d\xi, \dots (24 a)$

is an approximation to u_2 .

A value between 0 and 1 is then assigned to the constant γ in order to obtain the best possible approximation at small values of r. The first two terms in the expansion of f_1 are accordingly fitted to the corresponding terms in (11 a). It is found that $\gamma = \frac{2}{3} \exp(-\Psi(0))$.

In order to account for the pole of Ψ at the origin, f_1 and f_2 are calculated as appropriate to a modified potential curve which follows the tangent of the real curve at r_0 and has the value $2C/r_0$ at r=0. At $r=r_0$ the functions f_1 and u_1^* are joined and similarly the functions f_2 and u_2^* :

for $r < r_0$, $u_1 = u_1^*$, $u_2 = F_4 u_1^* + F_5 u_2^*$; for $r > r_0$, $u_1 = F_8 f_1 + F_9 f_2$, $u_2 = f_2$. The four constants are determined by four equations expressing continuity of the functions and their derivatives at r_0 .

Approximations to the solutions of (8b) are found similarly by means of the equation

$$v'' + [(2/r) - \Psi']v' - (2v/r^2) - [2h_1 - (1-\gamma)r](\Psi'v/rh_1) = 0, \dots (21 b)$$

the solutions of which are

$$h_1(r) = \frac{1}{3}r + \gamma r^{-2} \int_0^r [\exp \Psi(\xi) - 1] \xi^2 d\xi,$$
(20 b)

$$h_2 = qh_1$$
 $q(r) = -\int_r^{\infty} [\xi h_1(\xi)]^{-2} \exp \Psi(\xi) d\xi$ (24 b)

with $\gamma = \frac{1}{2} \exp(-\Psi(0))$, and the pole is accounted for in the same way as above. The function v_3 is equal to v_3^* for $r < r_0$ and is determined by (16) for $r > r_0$ with r_0 instead of 0 as lower limit of integration.

The present approximations, even without corrections for the pole, are sufficient for estimating the temperature effect. When better approximations are required they can be obtained by substituting the first approximation for the function in the last term of $(21\,a)$ and $(21\,b)$, adding the modified term to the right hand side and integrating by means of standard formulae.

§ 7. THE TEMPERATURE EFFECT

The coefficient of viscosity η and the coefficient of thermal conductivity λ are determined by expressions corresponding to those given in §4 of paper I:

$$\eta = -(N^2kT/aV)\int g_0 \Psi' u r^3 \sin^5 \theta \sin^2 2\phi \, dr \, d\theta \, d\phi, \quad \dots (25 a)$$

$$\lambda = -(N^{2}k^{2}T/2\beta mV) \int \{(r\Psi' - \Psi)[(v'/b) + \Psi + 1] \cos^{2}\theta + (\frac{1}{2}r\Psi' - \Psi)[(v/rb) + \Psi + 1] \sin^{2}\theta\}g_{0}r^{2}\sin\theta \,dr \,d\theta \,d\phi. \qquad \dots (25 b)$$

In (25 b) T_0 is replaced by T.

Viscosity is known to have a factor $\exp(U/kT)$ where U is an energy of the magnitude of the potential barrier outside the main minimum and $\exp(U/kT) \gg 1$. It is accordingly of interest to find out which solutions of $(6\,a)$ and $(6\,b)$ are of a magnitude similar to that of the exponential.

The integrand in (20 a) and (20 b) determining f_1 and h_1 is small at small values of r but increases exponentially outside the main minimum. Accordingly at large values of r the integrals are of the same magnitude as $\exp(U/kT)$. A lower limit for f_1 is derived from (20 a):

$$f_1 > \frac{1}{5}r^2 - \gamma r^{-3} \int_0^r \xi^4 d\xi = \frac{1}{2}(1 - \gamma)r^2$$
(26)

and a similar expression applies to h_1 .

The functions f_2 and h_2 are, according to (24a), (24b) extremely small at distances outside the barrier and reach the magnitude of unity only near the barrier. Their possible increase at the minimum is limited by the lower limit of f_1 and h_1 according to (26), so that their value is of a magnitude smaller than that of the exponential. Only at small values of r will the functions f_2 and h_2 increase exponentially.

The integrands in expression (16) determining the function v_3 have at no point the magnitude of $\exp(U/kT)$ so that the integrals do not reach this magnitude; v_3 itself is of the magnitude of the exponential at large values of r owing

to the factor $h_1(r)$.

In the integrands of (25 a) and (25 b) the functions u_1 , v_1 etc., are multiplied into g_0 . The high values of u_2 and v_2 near the origin and of the functions u_1 and v_1 near the barrier are offset by the negative exponential in g_0 . At large distances the high values of the functions u_1 and v_1 are ineffective because the integrand vanishes with Ψ' .

The transport coefficients can have accordingly an exponential temperature factor only if a constant of integration is proportional to a factor of this kind. These constants are determined by the constants in (9a), (9b). According to (20a), (20b) and considering the magnitude of the integrals in these expressions, only the constants F_2 and H_2 have the magnitude $\exp(U_k T)$. The constants F_1 and H_1 and, according to (14b) and (16), the constant H_6 are of smaller magnitude which by way of comparison may be said to be of magnitude unity. Determination of A_1 according to the boundary condition (18a) and of B_1 according to conditions (18b) shows that these constants have no exponential factor. B_2 vanishes according to (19b). Only the constant A_2 as determined by (19a) has an exponential factor which is peculiar to the viscosity of liquids. The characteristic difference of the temperature effect on the two transport coefficients is seen to be represented by the constants of integration.

§ 8. CONCLUSION

The effect of temperature on the transport coefficients as obtained in this paper is of a similar kind to that derived in paper I. The previous interpretation of the temperature effect is confirmed. In viscous flow the molecules are forced to occupy frequently positions of high potential energy whereas no such necessity is imposed on the molecules in the case of non-uniform temperature. In the first case the distortion of the equilibrium distribution is of higher magnitude than in the second.

The methods applied in this paper and in paper I may be regarded as different approximations to the exact theory. The present method no longer depends on the crude parabolic potential previously employed and can be adapted to the correct potential curve.

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Dislocation Theory of Yielding and Strain Ageing of Iron

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ABSTRACT. A theory of yielding and strain ageing of iron, based on the segregation of carbon atoms to form atmospheres round dislocations, is developed. The form of an atmosphere is discussed and the force needed to release a dislocation from its atmosphere is roughly estimated and found to be reasonable. The dependence on temperature of the yield point is explained on the assumption that thermal fluctuations enable small dislocation loops to break away; these loops subsequently extend and cause yielding to develop catastrophically by helping other dislocations to break away. The predicted form of the relation between yield point and temperature agrees closely with experiment.

Strain ageing is interpreted as the migration of carbon atoms to free dislocations. The rate of ageing depends upon the concentration of carbon in solution and the estimated initial rate agrees with experiment on the assumption that about 0.003% by weight of carbon is present in solution.

§ 1. INTRODUCTION

T was shown recently (Cottrell 1948) that the relief of stresses round a dislocation by foreign atoms in solid solution can cause an equilibrium "atmosphere" to form, in which large solute atoms are gathered in the dilated part of the dislocation field and small ones in the compressed part. An atom in substitutional solution relieves hydrostatic stresses and its interaction energy with a positive edge dislocation has been given as

$$V = \frac{4}{3} G \epsilon r_{\rm a}^3 \lambda \frac{1+\nu}{1-\nu} \frac{\sin \alpha}{r}, \qquad \dots (1)$$

where r and α are its coordinates relative to the dislocation, α being measured from the slip direction, G and ν are the rigidity modulus and Poisson's ratio respectively, λ is the slip distance in the dislocation, and $r_{\rm a}$ and $r_{\rm a}(1+\epsilon)$ are the respective atomic radii of solvent and solute. This formula fails at the origin because the elastic continuum theory is not valid in this region. To a first approximation, the dilatation is zero at the centre of a dislocation and it is reasonable to assume that V=0 when $r< r_0$, where $r_0 \sim \lambda$, and is otherwise given by equation (1).

In a dilute atmosphere the concentration of solute will be

$$n(r, \alpha) = n_0 \exp\{-V(r, \alpha)/kT\}, \qquad \dots (2)$$

where n_0 is the average concentration expressed as atoms per unit volume, but in a dense atmosphere substantial relaxation of the hydrostatic stresses is possible and an upper (saturation) limit of concentration is set by the condition that the local dilatations produced by the solute atoms and the field of the dislocation are everywhere equal and of the same sign.

Dislocations surrounded by atmospheres can produce plastic flow in two ways. If the applied force is small, the dislocations cannot escape from their atmospheres and the solute atoms must migrate with the dislocations. By applying a sufficiently large force, however, the dislocations can be torn from their atmospheres, in which case they then become highly mobile and able to produce rapid flow under smaller forces; a sharp upper yield point, followed by flow at a lower yield point, occurs. A specimen which is unloaded in this overstrained condition contains free dislocations and, on immediate reloading, shows no yield point, but if it is rested for a sufficient time at not too low a temperature before reloading, solute atoms migrate to the dislocations to form new atmospheres and the vield point returns (strain ageing). This type of hardening, caused by the assembly of mobile solute atoms round dislocations, is to be distinguished from the type of hardening considered previously in which dislocations are impeded by the strain fields of immobile irregularities, such as particles of precipitate. It is to be expected that, under suitable conditions, both types of hardening will be present simultaneously in the same material.

The yield phenomenon is particularly marked in mild steel and soft iron, where it is known to be associated with the presence of small amounts of carbon or nitrogen (Edwards, Phillips and Jones 1940, Snoek 1941b, Low and Gensamer 1944). Accordingly, it has been suggested (Cottrell 1948, Nabarro 1948) that the yield point of iron is due to carbon or nitrogen atmospheres. In the present paper this theory is examined by attempting to estimate the yield point and rate of strain ageing associated with carbon atmospheres; carbon is considered rather than nitrogen because it is more commonly present in iron, but the following discussion can be applied with very little modification to the case of nitrogen.

§2. CARBON ATMOSPHERES IN α-IRON

X-ray studies of martensite show that when carbon dissolves interstitially in α-iron it causes a marked lattice expansion and distorts the structure from cubic to tetragonal. These large strains must lead to a strong interaction between a carbon atom and a dislocation, which is consistent with the pronounced yield point of iron. In the case of a (positive) edge dislocation a carbon atom can relieve hydrostatic stresses by entering the expanded region below the dislocation centre; also, as was first pointed out by Nabarro (1948), an additional interaction can be expected because the non-symmetrical character of the distortion produced by carbon should enable shear stresses to be relieved. For a screw dislocation, Frank (1948) has suggested that the interaction must be due solely to the relief of shear stresses because hydrostatic stresses do not exist round a pure screw dislocation, so that in this case atmosphere formation can only occur with those solutes which, like carbon, produce a non-symmetrical distortion. The conditions for a given solute to be able to produce the yield phenomenon may thus be more stringent than was previously suggested, and a high mobility and a large degree of misfit, although necessary, may not in themselves be sufficient. However, considering the atomic structure in a screw dislocation in an actual metal lattice. it seems likely that the stress field will contain a small hydrostatic component, so that a weak interaction may exist with atoms which cause only spherically symmetrical strains.

The interstitial nature of the solution of carbon in iron and the non-symmetrical distortion prevent the use of equation (1) for calculating the interaction energy. Since the axis of the tetragonal distortion produced by a carbon atom is confined to one of the \$\leq 100 \rangle\$ directions of the body-centred cubic cell and a dislocation is confined to a slip-plane, with its direction of displacement lying in a slip direction, the system is not free to arrange that the tetragonal axis coincides with the direction of greatest tension in the dislocation field. For a complete analysis, therefore, the orientation and form of a dislocation in the iron lattice must be determined. The problem is much simplified if only the hydrostatic interaction is considered because hydrostatic stress is a scalar and the question of orientation is then avoided. In order merely to examine whether the anchoring force is sufficient to account for the yield point this simplification is justified and, accordingly, the present treatment deals only with the hydrostatic interaction with an edge dislocation. It is hoped to discuss the shear interaction in a later paper.

The interaction energy is determined by evaluating the work done by forces from the dislocation field when a lattice expansion occurs equivalent to the expansion caused by the introduction of a solute atom (Cottrell 1948). Assuming that each carbon atom alters the edges of the cell in which it is from a, a, a, to c, a_1 , a_1 , the mean changes in the lattice parameter produced by dissolving n carbon atoms in a crystal of N iron atoms are given by $\Delta c = 2(c-a)n/N$ and $\Delta a = 2(a_1 - a)n/N$. Using the lattice parameter measurements on martensite of Lipson and Parker (1944) and extrapolating to n/N = 0.5, the volume change caused by the introduction of a carbon atom is given as $\Delta v = 0.78 \times 10^{-23}$ cm³. Hence, if the stresses due to the dislocation in the surrounding medium remain constant when this local volume change occurs, the interaction energy is

$$V = p\Delta v = -q\Theta\Delta v \qquad \dots (3)$$

where p and Θ are the local pressure and dilatation, respectively, caused by the dislocation, and q is the bulk modulus. Using Koehler's (1941) formulae for the stresses round a positive edge dislocation

$$\Theta = -\frac{\lambda}{2\pi} \frac{1 - 2\nu}{1 - \nu} \frac{\sin \alpha}{r},$$

and assuming that $\Theta = 0$ when $r < r_0$ we have

$$V = A \frac{\sin \alpha}{r} = \Delta v \cdot \frac{G\lambda}{3\pi} \frac{1+\nu}{1-\nu} \frac{\sin \alpha}{r} \quad r \geqslant r_0; \qquad V = 0 \quad r < r_0.$$
....(4)

The assumption that the dislocation stresses, and hence Θ , remain unchanged when the carbon atom is introduced implies that the stress field is effectively constant over regions large compared with the size of the carbon atom, a reasonable approximation in regions remote from the dislocation centre. Near the centre, however, the dislocation stresses are rapidly varying functions of position and must be greatly altered by the introduction of the carbon atom. In the part of the crystal below the dislocation (i.e. where Θ is positive), which is the region of interest for the case of carbon in iron, the (negative) pressure must relax as the local volume change Δv takes place so that the interaction energy will be less

than is given by equation (4). Very near the dislocation centre equation (4) will grossly overestimate the interaction and can only be used to give a rough

indication of the general order of magnitude.

Taking $G=8\cdot28\times10^{11}$ dyne.cm⁻², $\lambda=2r_{\rm a}=2\cdot48\times10^{-8}$ cm., and $\nu=0\cdot28$, the constant A in equation (4) is 3×10^{-20} dyne.cm². At room temperature A kT=76 Λ . and, with such a value, the Maxwell-Boltzmann formula (2) gives impossibly large values of n n_0 in the lower half crystal within about 10 Λ . of the dislocation centre. The concentration in this region must be limited by other factors. An assembly of carbon atoms can never completely relieve all the dislocation stresses, but, as the atmosphere builds up, the progressive relief of stress will lead to a condition of saturation in which the addition of more atoms to the atmosphere no longer reduces the energy. An estimate of the number of atoms required for saturation can be made by equating the volume changes produced by the atoms and by the dislocation field. Taking a section consisting of one atomic plane threaded by the dislocation line, the radius R of a semicircular annulus, in which the total volume change produced by the dislocation is equal to that produced by introducing one carbon atom, is determined by

$$\Delta v = \lambda \int_{r_0}^{R} \int_{\pi}^{2\pi} \Theta r \, dr \, d\alpha.$$

Using the above value for Δv and assuming $r_0 \sim 2\,\mathrm{A}$. R is about 10 A. It is thus reasonable to assume that in the equilibrium state only one carbon atom per atom plane is contained within 10 A. of the dislocation centre. Since the greatest tensile strain must occur immediately below the dislocation centre and in the atomic plane which constitutes the lower side of the slip plane, the most favourable position for the central carbon atom will be at $\alpha = 3\pi/2$ and $r \sim 2\,\mathrm{A}$., and it seems likely that the central part of the atmosphere consists of a line of carbon atoms, parallel to the dislocation line, in this position. In the annulus between 10–20 A. the total volume change is again about the same as that produced by one carbon atom per atom plane, but this volume change is spread more uniformly over a much larger region of the crystal and, in this case, the carbon atoms could hardly be arranged along a line. The atmosphere is pictured, therefore, as a central row of carbon atoms, situated just below the dislocation centre, which is surrounded in the lower half-crystal by a dilute distribution of the Maxwell-Boltzmann type.

It should be noticed that an extremely small amount of carbon is required to provide atmospheres for all dislocations in a crystal; the actual value depends,

Table 1

Density of dislocation (lines/cm ²)	1012	108
% of C by weight absorbed full yield point	$ > 10^{-2}$	>10-6
in dislocations for \(\bigcap\) No yield point	$ < 10^{-3}$	$< 10^{-7}$

of course, on the density of dislocations. Table 1 shows the results of the assumption that a full yield point is obtained when every dislocation has one carbon atom per atom plane and that the yield point is absent at below one-tenth of this amount of carbon.

§ 3. FORCE REQUIRED TO PULL A DISLOCATION FROM ITS ATMOSPHERE

It is clear that the force required to pull a dislocation from its atmosphere is determined almost completely by the interaction with the carbon atoms of the central row, since (i) these atoms, being so near to the dislocation, interact strongly with it, and (ii) the restraining force due to their interaction must reach its maximum at a very small displacement of the dislocation from its equilibrium position, and at such a small displacement the contribution to the restraining force from carbon atoms further out will still be comparatively small. From the point of view of calculating the yield point this is unfortunate, since it means that the important contribution of force is from atoms near the dislocation centre, where the interaction energy cannot be accurately evaluated, so that only a rough estimate is possible.

In Figure 1 consider a positive edge dislocation lying along the Z axis (the X axis is the slip direction) and a line of carbon atoms CC', lying parallel to the dislocation, in the most favourable position at a distance ρ below it. The interaction energy per atom plane, when the dislocation has been displaced a distance x in the slip direction is

$$V(x) = -A \sin \phi / r = -A\rho/(x^2 + \rho^2) \qquad \dots (5)$$

and the corresponding force is $F(x) = \frac{\partial V}{\partial x} = \frac{2A\rho x}{(x^2 + \rho^2)^2}$ which has a maximum of $3\sqrt{3}A/8\rho^2$ dynes per atom plane at $x = \rho/\sqrt{3}$.

The critical force for releasing a dislocation is thus $F_0=3\sqrt{3A/8\lambda\rho^2}$ dynes/cm. and, by using the relation $\tau=F/\lambda$ (Mott and Nabarro 1948) where τ is resolved shear stress, this can be converted to an equivalent critical shear stress $\tau_0=3\sqrt{3A/8\lambda^2\rho^2}$ dyne.cm⁻² on the slip plane. Assuming that in the case of a tensile test the active slip planes are inclined at approximately $\pi/4$ to the tensile axis, the critical tensile stress is

$$\sigma_0 = 3\sqrt{3}A/4\lambda^2\rho^2$$
 dyne.cm⁻².(6)

Table 2 gives the observed values of the yield point of annealed ingot iron at various temperatures, as derived from the graphical results of McAdam and Mebs (1943). The yield shows a strong temperature dependence and it is clear

Table 2

Temperature (° K.)	85	144	195	303	373
Yield point σ (dynes/cm ² × 10 ⁹)		4.14	2.83	1.45	1.10
σ/σ_0		0.330	0.225	0.115	0.090

that σ_0 in equation (6) must correspond with the zero point yield stress. If a curve is fitted to these results and extrapolated to 0° K., the experimental value of σ_0 is about 1.25×10^{10} dynes/cm². Using the precious values of A and λ the theoretical value of σ_0 can be made to agree with this if ρ is taken to be 7 A., which shows that the restraining force is strong enough to account for the yield point. If ρ is taken to be 2 A., as suggested in §2, the estimated value of σ_0 is an order of magnitude higher; however, it must be remembered that the interaction energy is seriously over-estimated near the dislocation centre and the theory can only give a rough indication of the yield stress. Comparison with the experimental value of σ_0 suggests that a reasonable value of A near the dislocation centre is 3×10^{-21} dyne.cm².

Figure 2 shows the variation of interaction energy and stress with position of the dislocation for the cases $\rho = 2 \,\text{A.}$, $A = 3 \times 10^{-20} \,\text{dyne.cm}^2$, and $\rho = 2 \,\text{A.}$, $A = 3 \times 10^{-21} \,\text{dyne.cm}^2$.

§ 4. EFFECT OF THERMAL FLUCTUATIONS ON THE YIELD POINT

At temperatures above 0° K., thermal fluctuations help the external forces to tear a dislocation from its atmosphere and yielding occurs before σ reaches σ_0 . When a stress $\sigma = p\sigma_0$ is applied the dislocation moves forward to the position x_1 of stable equilibrium (Figure 2) and can only be released by this stress after it has been taken further forward to the position x_2 of unstable equilibrium, beyond which the external force exceeds the restraining force.

The activation energy per atom plane for the release, by thermal fluctuations, of a dislocation which remains straight is thus the difference $V(x_2) - V(x_1)$ in

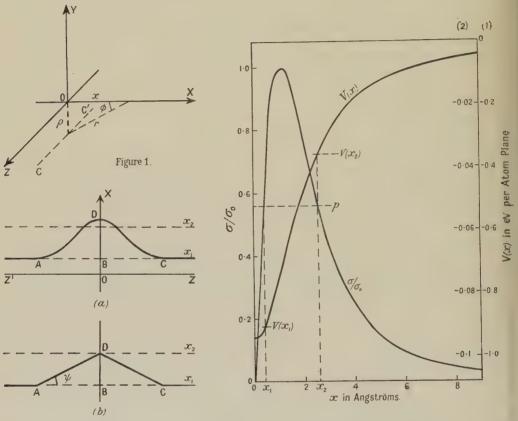


Figure 3.

Figure 2. Variation of interaction energy (V) and applied stress (σ/σ_0) with dislocation position.

Scale (1) $A = 3 \times 10^{-20}$ erg.cm. $\rho = 2$ A. Scale (2) $A = 3 \times 10^{-21}$ erg.cm. $\rho = 2$ A.

interaction energy minus the work done by the external force when the dislocation moves from x_1 to x_2 . In calculating the activation energy which thermal fluctuations must supply in order to release the whole dislocation, however, an energy contribution caused by the change in form of the dislocation must be considered.

Let the plane of Figure 3(a) represent the slip plane. When the applied stress is zero the equilibrium position of the dislocation is ZZ', vertically above the line of the atmosphere. Under the stress σ the dislocation moves forward to the line x_1 . To produce yielding it is not necessary for the fluctuation to

move the entire dislocation to x_2 as this would require an unnecessarily large energy. If a loop ADC of the dislocation is thrown forward, and this loop is sufficiently large, the force pulling the looped part forward can exceed the restraining force and the dislocation will then be torn from its atmosphere, the centre of the loop moving forward and the sides moving laterally towards the ends of the dislocation. This process depends upon the ability of the dislocation to be bent and extended. The theory of flexible dislocations has been developed by Mott and Nabarro (1948) who have shown that a dislocation behaves like a one-dimensional soap film; it possesses an energy WL, where L is its length and W=1-5 ev. per atom plane, which it tries to minimize by becoming as short as possible. Thus to form the loop ADC, an activation energy has to be supplied which is made up of (i) the energy of interaction with the atmosphere, (ii) the length energy associated with the increase in length, ADC-ABC, and (iii) the energy gain due to the work done by the external forces.

To calculate the exact size and shape of the smallest stable loop is difficult, but it is clear that an essential condition is that part of the dislocation has to be brought by the fluctuation to at least the line x_2 , since otherwise there will be no part of the looped dislocation on which the net force acts in the forward direction. Thus consider the simpler model shown in Figure 3 (b). Here a triangular loop is formed, of depth BD, reaching to the line x_2 at its apex, and the value of the angle ψ is chosen to make the activation energy a minimum. This loop is, of course, too small to be stable; however, the true activation energy cannot be very much greater than is given by this model, for calculation shows that about one-half of the energy of the triangular loop arises from the length energy term and much larger loops could be formed with only a small additional increase in the length of the dislocation.

It is assumed that the interaction energy of an element at any point on the portions AD and DC is the same as that of an element with that point as centre and lying parallel to ZZ'; this assumption is consistent with the results of the analysis by Mott and Nabarro (1948) of the strains round a zigzag dislocation. Accordingly, when an element dz of the dislocation moves forward from x_1 to x, with the formation of the loop, its interaction energy changes by

$$\{V(x) - V(x_1)\} dz = -\cot \psi \{V(x) - V(x_1)\} dx$$

and the contribution of the interaction with the atmosphere to the activation energy is

$$2\int_{x_0}^{x_1} -\cot\psi\{V(x) - V(x_1)\}\,dx.$$

Taking $V(x) = -A\rho/\lambda(x^2 + \rho^2)$ erg/cm. this becomes

$$-\left[\frac{2A}{\lambda}\left\{\tan^{-1}(x_{2}/\rho)-\tan^{-1}(x_{1}/\rho)\right\}+2(x_{2}-x_{1})V(x_{1})\right]\cot\psi.$$
 (7)

The increase in length energy is

$$W(ADC - ABC) = 2W(x_2 - x_1)(\csc \psi - \cot \psi) \qquad \dots (8)$$

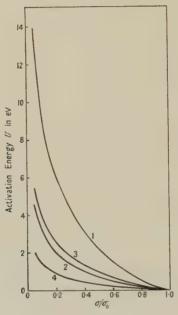
and, if the external force per unit length on the dislocation is F, the work it does when the loop is formed is

$$F(x_2-x_1)^2\cot\psi. \qquad \dots (9)$$

Subtracting (9) from the sum of (7) and (8) gives the activation energy, U, which is of the form $\alpha \csc \psi - \beta \cot \psi$; minimizing U with respect to ψ defines ψ as $\cos^{-1}(\beta/\alpha)$ and substituting this value then gives the activation energy in terms of W and σ/σ_0 . It can be readily shown that U is of the form

$$U = D(\sigma/\sigma_0)[AE(\sigma/\sigma_0)\{2W\rho - AE(\sigma/\sigma_0)\}]^{\frac{1}{2}},$$

where D and E do not depend on the physical parameters A, W and ρ . Thus, if $2W\rho \gg AE$, $U(2AW\rho)^{\frac{1}{2}}$ is essentially a function of σ/σ_0 only, so that altering A, W and ρ only alters the curve of U against σ/σ_0 by a scale factor, the form of the curve remaining unchanged. For the range of values of A, W, ρ and σ/σ_0 considered, AE is never greater than about $W\rho/2$ and in most cases is much less than this, so that the form of the activation energy curve is almost independent of the parameters. Figure 4 shows the curve for various values of A, W and ρ .



It is to be expected that, as the stress is increased towards σ_0 , the first successful attempt to form a loop occurs on a dislocation in a highly stressed region of the specimen. The first stable loop to be formed is subsequently extended by the applied force until the entire dislocation to which it belongs is released from its atmosphere. This dislocation accelerates and enables other dislocations to break away by setting up an elastic disturbance in their midst; in this way yielding develops catastrophically throughout the entire specimen. This description agrees with the well-known observations that yielding starts in highly stressed regions and is propagated, in the form of Luder's bands, from these regions along the specimen. The elementary yielding process—the release of a dislocation from its atmosphere—occurs in both the start and the propagation of yielding; the difference between the upper and lower yield points is that, in the case of the

lower yield, the release of dislocations (at the edges of a Luder's band) is helped by the elastic disturbance caused by nearby plastic flow, whereas in the upper yield this help is not available.

With the above picture the effects of temperature and testing rate on the yield point can be examined. When the stress in the neighbourhood of a dislocation lies in the range σ/σ_0 to $(\sigma+d\sigma)/\sigma_0$ the time t_1 before a successful fluctuation occurs is proportional to $\exp\{U(\sigma/\sigma_0)/kT\}$. On the other hand, the time t_2 spent in this stress range is inversely proportional to the rate of stressing, $d\sigma/dt$. Yielding should occur when $ts \sim t_2$, i.e. when the quantity

$$S = (d\sigma/dt) \exp\{-U(\sigma/\sigma_0)/kT\} \qquad \dots (10)$$

reaches a characteristic, fixed value. Thus, in experiments at constant testing rate, the yield point should vary with temperature in such a manner that U/kT remains constant, and similarly, at constant temperature U should depend logarithmically on the testing rate. From McAdam and Mebs' results (Table 2) the temperature dependence can be examined. If the experimental and theoretical values of σ/σ_0 are equated at one arbitrarily chosen temperature, the value of U and hence U/kT can be found from Figure 4. Keeping U/kT constant the theoretical σ/σ_0 values can be obtained at various temperatures from Figure 4 and compared with the experimental values. Figure 5 shows the results obtained

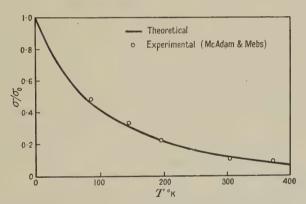


Figure 5. Variation of yield point with temperature. The theoretical curve is fitted to the experimental value of σ/σ_0 at 195° K.

when the σ/σ_0 values are equated at 195° K. and the activation energy curve 4 of Figure 4 is used. Since the activation energy curves have almost identical forms essentially the same results are obtained when the other curves are used. The good fit obtained over a wide range shows that the activation energy curves

	Ta	able 3			
Activation energy curve		1	2	3	4
W (ev. per atom plane)		. 5	5	1	1
A (dyne.cm ² × 10 ⁻²⁰)		3	0.3	3	0.3
U/kT		330	107	140	47

have the correct shape to account for the experimental observations. The values of U/kT given by equating the σ/σ_0 values are shown in Table 3. Since U/kT in practice could hardly exceed about 50, it appears that the most reasonable values of W and A are those of curve 4.

In the present theory, the large temperature dependence of the yield point of iron is explained by the narrowness of the potential energy trough associated with an atmosphere of solute atoms (cf. Figure 2), so that only a small displacement of the dislocation, and hence a small activation energy, is required to overcome the restraining force. In a precipitation-hardened alloy, on the other hand, the existence of wide potential energy troughs causes a large activation energy for moving a dislocation, thus giving a small temperature dependence of yield strength (Mott and Nabarro 1948).

§ 5. RATE OF FORMATION OF THE ATMOSPHERE

In the present theory, strain ageing is regarded as the process whereby carbon atoms in solution migrate towards free dislocations, at rest in an overstrained crystal, to form new atmospheres. To examine this process consider a free dislocation at rest in a region where the solute is initially randomly dispersed, with concentration n_0 atoms per cm³. Moving by thermal agitation the solute atoms acquire a drift velocity relative to the dislocation (Cottrell 1948) given by

$$\mathbf{v} = -(D/kT)\nabla V \qquad \dots \dots (11)$$

where D is the diffusion coefficient and V is given by equation (4). As the atmosphere builds up to equilibrium, both saturation and concentration differences become important in modifying the flow velocity, but in the early stages of atmosphere formation they are negligible. As it is extremely difficult to take account of these factors quantitatively, only the initial stages of ageing, where the drift flow is dominant, will be considered.

Equation (11) shows that the atoms move normally to the equipotential surfaces of V. It is thus convenient to choose as coordinate lines for the problem an orthogonal, curvilinear set consisting of the families made up from the lines of constant V and the lines of flow; the problem is, of course, two-dimensional. Since $V = A \sin \alpha / r$, the first coordinate may be defined by the parameter $\eta = r/\sin \alpha$, so that the equipotential lines are those on which η is constant. The flow lines, conjugate to these, are defined by the coordinate $\xi = r/\cos \alpha$. Using the standard transformation formulae, the elements of length along the ξ and η lines are, respectively,

 $\frac{\xi^2}{\xi^2 + \eta^2} d\eta \quad \text{and} \quad \frac{\eta^2}{\xi^2 + \eta^2} d\xi \qquad (12)$

and ∇V is

$$-A\frac{\xi^2+\eta^2}{\xi^2\eta^2}\mathbf{i},\qquad \qquad \dots (13)$$

where **i** is the unit vector in the η direction. As shown in Figure 6, the ξ , η coordinate system consists of circles centred on the X, Y axes and passing through the origin.

A carbon atom will migrate towards the most favourable position below the dislocation, moving along a line of constant ξ and eventually come to rest at a position where its η coordinate has a value, $-\eta_0$, of a few Angströms. From (11), (12) and (13), the time required for an atom to move an elementary distance in the η direction is

$$dt = \frac{kT}{AD} \frac{\xi^4 \eta^2}{(\xi^2 + \eta^2)^2} d\eta,$$

and hence the time to move from $(\xi, +\eta_0)$ to $(\xi, -\eta_0)$ is

$$\begin{split} t &= \frac{kT}{AD} \, \xi^4 \bigg(\int_{+\,\eta_0}^{+\,\infty} \big\{ \eta^2 \, d\eta / (\xi^2 + \eta^2)^2 \big\} \, + \, \int_{-\,\infty}^{-\,\eta_0} \big\{ \eta^2 \, d\eta / (\xi^2 + \eta^2)^2 \big\} \bigg) \\ &= (kT \xi^3 / AD) \big[\pi / 2 - \tan^- \big(\eta_0 / \xi \big) + \frac{1}{2} \sin \big\{ 2 \, \tan^{-1} (\eta_0 / \xi) \big\} \big]. \end{split}$$

If $\eta_0/\xi \ll 1$ this can be approximated to

$$t = \pi k T \xi^3 / 2AD \qquad \dots (14)$$

since $\tan^{-1}(\eta_0/\xi) \sim \frac{1}{2} \sin \{2 \tan^{-1}(\eta_0/\xi)\} \sim \eta_0/\xi$. After the time t, all lines of flow for which $\xi^3 \le 2ADt/\pi kT$ will have been drained of carbon atoms and will take no further part in the ageing process. Taking the smallest value of ξ compatible with the above approximation to be $10 \,\mathrm{A.}$, and using the value of §2 for A/kT,

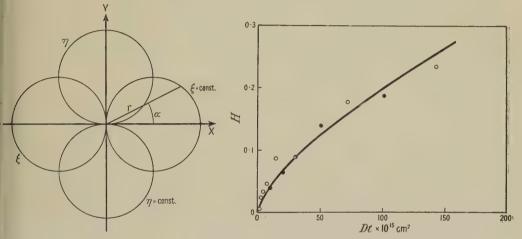


Figure 6.

Figure 7. Strain ageing of a low-carbon steel. (From results of Davenport and Bain.)

 \bigcirc = Ageing at 20° c.

=Ageing at 40° C. =Equation (16) assuming a carbon concentration of 0.003 % by weight.

it can be seen that this conclusion should be valid for ageing times such that $Dt > 2 \times 10^{-15}$ cm². As Figure 7 shows, strain ageing does not become appreciable until much longer ageing times than this have elapsed.

Consider flow along a filament of width $d\xi$ which is still supplying atoms at the time t. The time for an atom to move an elementary distance along this filament, in the region where $\eta = -\eta_0$, is

$$dt = \frac{kT}{AD} \frac{\xi^4 \eta_0^2}{(\xi^2 + \eta_0^2)^2} d\eta$$

and the area of the corresponding element of the filament is

$$\frac{\xi^2\eta_0^2}{(\xi^2+\eta_0^2)^2}\,d\eta\,d\xi = \frac{AD}{kT}\frac{d\xi}{\xi^2}\,dt.$$

Using equation (14) to define the limits of integration, the total area which can supply carbon atoms to the dislocation in the interval of time from t to t+dt is

$$\frac{AD}{kT} \left(\int_{+(2ADt/\pi kT)^{\frac{1}{8}}}^{+\infty} \xi^{-2} d\xi + \int_{-\infty}^{-(2ADt/\pi kT)^{\frac{1}{8}}} \xi^{-2} d\xi \right) dt = 2 \left(\frac{\pi}{2} \right)^{\frac{1}{8}} \left(\frac{AD}{kT} \right)^{\frac{8}{8}} \frac{dt}{t^{\frac{1}{8}}} \dots (15),$$

An important feature is that, in the region of the dislocation field where the relation $V=A\sin\alpha_/r$ holds, and outside the regions defined by equation (14) from which the carbon atoms have been removed, the concentration of carbon remains constant during the drift flow. The hydrodynamical equation of continuity, $\nabla \cdot (\rho \mathbf{v}) = -\partial \rho/\partial t$, here takes the form $\nabla \cdot \{n(D/kT)\nabla V\} = \partial n/\partial t$ where $n=n(r,\alpha,t)$ is the concentration of solute. Since $n=n_0=$ constant at t=0, and since $\nabla^2 V = (\partial^2/\partial r^2 + \partial/r\partial r + \partial^2/r^2\partial\alpha^2)(A\sin\alpha/r) = 0$ then $\partial n/\partial t = 0$ and the condition $n=n_0$ is perpetuated.

If unit length of the dislocation is considered, the number of carbon atoms which arrive within a time t is, from equation (15),

$$N(t) = n_0 2 \left(\frac{\pi}{2}\right)^{\frac{1}{8}} \left(\frac{AD}{kT}\right)^{\frac{2}{3}} \int_0^t t^{-\frac{1}{8}} dt = n_0 3 \left(\frac{\pi}{2}\right)^{\frac{1}{8}} \left(\frac{ADt}{kT}\right)^{\frac{2}{8}}.$$

The total number, N_s , of carbon atoms per unit length of the dislocation required to form an atmosphere of one atom per atom plane is $1/\lambda$, so that the degree of formation of the atmosphere at time t is

$$N(t)/N_{\rm s} = n_0 \lambda 3(\pi/2)^{\frac{1}{3}} (ADt/kT)^{\frac{2}{3}}.$$
(16)

§6. RATE OF STRAIN AGEING

An experimental study of strain ageing has been made by Davenport and Bain (1935) who measured the increase in hardness of a low-carbon steel with time of ageing at various temperatures. Nabarro (1948) has shown that several features of strain ageing, shown by their results, are explicable on the basis of the present theory and provide evidence in its support. To compare the ageing rates found by Davenport and Bain with the rate predicted in the previous section the quantity $H = (H_t - H_0)/(H_m - H_0)$ which is a measure of the degree of strain age-hardening, is first derived from the graphical results given in their Figure 11 (upper block); in this expression, H_t is the hardness after ageing for a time t, H_0 is the value before ageing and H_m is the maximum produced by prolonged ageing. To assemble results from different temperatures in the same diagram it is convenient to plot H against Dt rather than the time t itself, where $D = 5.2 \times 10^{-4} \, e^{-9000/T}$ (Snoek 1941a, Polder 1945) is the diffusion coefficient of carbon in α -iron, since all the results then lie on the same curve.

Figure 7 shows the experimental and theoretical variation of H with Dt. The theoretical curve has been derived from equation (16) by assuming that $H=N(t)/N_s$, by using the values of λ and A/kT given in §2, and by taking a value of n_0 corresponding to 0.003% carbon by weight. The assumption $H=N(t)/N_s$ cannot be strictly valid since the first atoms to arrive at a dislocation ought to be more effective in anchoring it than those that arrive later. Equation (16) represents the observed ageing behaviour fairly well up to about $N(t)/N_s=0.3$ but beyond this range it gives a rate of ageing which is too high; this is to be expected since the neglect of the effects of saturation and concentration differences, and the assumption $H=N(t)/N_s$, will each cause the theoretically estimated rate to be too high in the later stages of ageing.

The carbon concentration determined above by fitting the observed and calculated ageing rates ought to correspond to the value for the residual carbon

in solution in α -iron at room temperature. Most of the carbon in irons and steels of higher carbon content is, of course, precipitated as cementite and only that which remains in solution takes part in strain ageing. Experimental evidence for the solubility of carbon in iron at room temperature is meagre, but suggests that the above value of 0.003% is reasonable. Thus Yensen (1924) and Dijkstra (1947) have given the upper limit of the residual solubility as 0.006% and 0.001% respectively.

§7. OTHER AGEING EFFECTS

The migration of solute atoms into dislocations, causing the latter to become anchored, ought to produce several mechanical and physical effects, which can be divided into two groups: (i) those resulting from the anchoring of the dislocations, and (ii) those resulting from the removal of solute atoms from random solution to form atmospheres.

The most striking effect belonging to the first group is, of course, the return of the yield point. In addition, a reduction of certain "anelastic" effects (Zener 1946) is to be expected, and this is confirmed by experiment. A freshly strained specimen possesses a high internal friction and shows slight plasticity at stresses well below the stress at which extensive plastic flow sets in. Zener has attributed these anelastic effects to local readjustments in position of dislocations in the slip bands of the worked material; this is reasonable since small displacements of free dislocations in a Taylor (1934) array can occur under small stresses, even though a high stress is required to overcome the interaction forces of neighbouring dislocations and so produce extensive flow. Low-temperature annealing, for times which would allow strain ageing to occur, greatly reduces this source of internal friction and causes a true elastic range to return, which is consistent with the suggestion that dislocations become anchored by the ageing process.

Ageing effects belonging to the second group should be provided by properties which are sensitive to the amount of carbon in random solution in α -iron. Thus we may expect both electrical resistance and magnetic ageing effects. Recent work by Mr. A. T. Churchman and one of us (A. H. C.) has shown that a small decrease in electrical resistance of the right order of magnitude does in fact occur during strain ageing. Another effect has been observed by Snoek (1941a), who found that cold working and low-temperature annealing caused the elimination of a certain type of elastic after-effect known to be caused by mobile carbon (or nitrogen) atoms in solution in α -iron. Snoek suggested that this treatment probably caused the solute atoms to become bound by internal stress fields created by the cold working. If we interpret the sources of the stress fields as dislocations, this suggestion becomes quite specific, since then the solute atoms cannot produce internal friction by Snoek's mechanism because they are assembled in dislocations.

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Investigations on the Binding Energy of Heavy Nuclei

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ABSTRACT. The binding energy of a heavy nucleus is one of the quantities which a satisfactory nuclear force theory ought to predict correctly. Approximate calculations of this binding energy are performed, taking as nuclear force the static interaction of Møller and Rosenfeld. The parameters appearing in the interaction have been fixed by data on light nuclei.

The Fermi-gas model is taken as basis for the calculations, a first solution being obtained by a first-order perturbation (or variation) method. For refinement, a second-order perturbation calculation is made, and Svartholm's variation-iteration method is attempted. The first-order results yield about 10% of the required energy, and the second-order about 40%; a reasonable prediction of the size of the nucleus is obtained. The reliability of the perturbation results is uncertain; Svartholm's method does not appear to be well suited to the investigation of heavy nuclei.

Two alternative modifications are made to the nuclear force to make it yield the correct binding energy according to the perturbation calculation.

§ 1. INTRODUCTION

In principle, one of the most important tests of any proposed nuclear force is its compatibility with the observed binding energies of heavy nuclei. By a semi-empirical procedure these can be approximately expressed by a simple function of atomic number Z and mass number A, containing a few parameters. One of these parameters, the coefficient of an energy contribution simply proportional to A, can be taken as representing the major effect of the nuclear forces, and a theory might be tested by the value which it predicts for this parameter. Of the theories which have been put forward, that of Møller and Rosenfeld (Møller and Rosenfeld 1940, Rosenfeld 1945, 1948) is capable of accounting for many of

the properties of light nuclei, and is at the same time relatively easy to handle: this is the theory here considered in relation to heavy nuclei. The parameters appearing in the interaction are fixed by data on light nuclei. The problem posed is the solution of the wave equation for the ground state of a very heavy nucleus. Approximate methods must be employed for this, and in consequence the reliability of the test cannot very well be assessed.

The methods used are based on the Fermi gas model (§ 3.1), a first approximate solution being obtained by a first-order perturbation (or variation) treatment (§ 3.2). Two different possibilities of refinement have then been attempted, viz. a second order perturbation calculation (§ 3.3), similar to that first performed by Euler (1937) for a different form of interaction; and Svartholm's variation-iteration method (§ 5). The former leads to positive results, but it appears that Svartholm's method is not well suited to the investigation of heavy nuclei. The results of the perturbation calculations are presented in § 2, and the calculations are criticized in § 4.

§ 2. FORMULATION OF PROBLEM AND RESULT

2.1. Formulation of Problem

The binding energy -E of a nucleus of atomic number Z and mass number A can be represented approximately by the semi-empirical formula (Rosenfeld 1948, Chap. 2)

$$E = -c_1 A \left[1 - c_2 \left(\frac{N - Z}{A} \right)^2 \right] + c_3 A^{\frac{3}{2}} + \frac{3}{5} \left(\frac{e^2}{r_0} \right) \frac{Z^2}{A^{\frac{1}{2}}}, \qquad \dots (1)$$

where c_1 , c_2 , c_3 are constants, N is the number of neutrons, A-Z, and r_0 is the radius of the sphere whose volume is that occupied by one nucleon, viz:

$$r_0 = (\text{radius of nucleus})/A^{\frac{1}{3}}$$
.

 r_0 is observed to be approximately constant, and is taken to be exactly so in equation (1).

The several terms in the formula have the following significance: The first (if c_2 is neglected) represents the bulk of the "nuclear forces" binding the nucleus. The factor containing c_2 is a correction for disparity in the numbers of neutrons and protons. The second term is a "surface-tension" effect, and the last term represents the electrical energy of repulsion of the protons.

We are chiefly concerned with the parameter c_1 , whose observed value, found by fitting equation (1) to the nuclear energy surface, is to be compared with that predicted theoretically. By extrapolation of equation (1), c_1 may be interpreted as the binding energy per nucleon of an "ideal" nucleus, i.e. an assembly of an infinite number of neutrons and protons in equal proportions, if the electrical repulsion between the protons is removed. r_0 can also be estimated theoretically and compared with the observed value.

For the theoretical analysis the static interaction of Møller and Rosenfeld (Møller and Rosenfeld 1940, Rosenfeld 1945, 1948) is employed. At this point, dimensionless variables, to be used throughout, are introduced, by setting up the following "absolute" units:—

Unit of mass—mass M of a nucleon (proton and neutron being assumed equally heavy). Unit of length—range of nuclear force,
$$1/\lambda$$
; defined by $\lambda = \mu c/\hbar$ where $\mu = \text{mass}$ of meson. Unit of angular momentum— \hbar .

These yield the derived "absolute" unit:

Unit of energy—
$$Mc^2(\mu/M)^2 = \lambda^2 \hbar^2/M$$
.(3)

Then in these units, any pair of nucleons i and j has the mutual potential

$$w_{ij} = (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)[g^2 + f^2(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)] \exp(-\xi_{ij})/\xi_{ij}, \qquad \dots (4)$$

where σ_i and τ_j are the spin and isotopic operators respectively for the i-th nucleon, ξ_{ii} is the separation of the nucleons, and g and f are interaction constants.

The values of the parameters μ , f and g are taken from Fröhlich *et al.* (1947, equation (76)), where they were chosen so as to fit correctly the two lowest energy levels of the neutron–proton system and the ground level of H^3 :

$$\mu = 220 \text{ m.}; \quad f^2 = 0.595; \quad g^2 = 0.258. \quad \dots (5)$$

These make the unit length, $1/\lambda$, equal to 1.75×10^{-13} cm.; and the unit of energy equal to 14.4 m.m.u., or 13.4 mev.

The observed values assumed for the quantities c_1 and r_0 of equation (1) are those given by Bethe and Bacher (1936, § 30), viz. $c_1 = 14.9$ M.M.U. (1.03 in absolute units), $r_0 = 1.48 \times 10^{-13}$ cm. (0.85 in absolute units).

2.2. Results

The "ideal" nucleus is subjected in § 3.2 to a variation treatment, on the basis of the Fermi-gas model. This yields a value of the binding energy per nucleon for each initially arbitrarily assumed size of the nucleus. Minimization of the energy with respect to the size yields estimates of both the actual binding energy and the actual size.

In Figure 1 are plotted the expectation values of the kinetic, potential and total

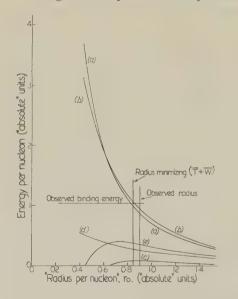


Figure 1. Energies per nucleon calculated on Fermi-gas model, vs r_0 , representing size of nucleus.

(a)
$$\overline{T}|A$$
; (b) $\overline{W}|A$; (c) $(\overline{T}+\overline{W})|A$; (d) $E''|A$; (e) $(\overline{T}+\overline{W}+E'')|A$.

The kinetic energy \overline{T}/A (curve (a)) and potential energy \overline{W}/A (curve (b)) almost cancel. The maximum binding energy $-(\overline{T}+\overline{W})/A$ by the variation (first order perturbation) method is far below the observed value: the radius r_0 which minimizes $(\overline{T}+\overline{W})$ is in good agreement with the observed value.

The second order perturbation energy E''/A (curve (d)), when added to $(\overline{T}+\overline{W})/A$ (curve (e)), raises the binding energy considerably, but it is still well below the observed value for all r_0 .

energies (curves a,b,c, respectively) per nucleon as functions of r_0 , the "radius per nucleon". At the minimum of the total energy it is found that the kinetic energy per nucleon $=\overline{T}/A=0.97$, the potential energy per nucleon $=\overline{W}/A=-1.06$, and therefore total energy per nucleon =-0.09. (All energies are expressed in the absolute units of equation (3)). The binding energy is thus of a smaller order of

magnitude than the value 1.03 required, as in the case of similar calculations previously carried out with different forms of interaction (Bethe and Bacher 1936, p. 157, Rosenfeld 1948). The minimizing radius r_0 is equal to 0.90 (in the absolute unit of equations (2)), which compares well with the observed value 0.85.

Although the binding energy obtained is so small, it may be noted that a quite moderate increase in the strength of the potential would increase it rapidly, because the potential and kinetic energies under the assumed conditions almost cancel.

The second order perturbation calculation, which is carried out in §3.3, yields a term E'' to be added to the former energy $(\overline{T}+\overline{W})$. The energy is again found for variable size of the nucleus; although perturbation theory does not strictly prescribe what size will give the best prediction for the energy $(\overline{T}+\overline{W}+E'')$, the minimum of the latter quantity with respect to size was taken as being probably as good as any. However, there seems no reason in principle why the corresponding minimizing radius r_0 yielded by the second order calculation should be any better as an approximation to the actual radius than that yielded by the variation calculation. The latter has therefore been retained as the theoretical prediction of the radius r_0 .

Graphs of E''/A and the total energy $(\overline{T}+\overline{W}+E'')/A$ are shown in Figure 1, curves (d) and (e). It will be seen that |E''| is much larger than $|\overline{T}+\overline{W}|$ at all radii, indicating that the variation treatment is extremely poor. The minimal value of the total energy per nucleon is found to be -0.41. This is much better than before, but still falls far short of the required value -1.03. This second result, then, indicates that the Møller-Rosenfeld interaction is too weak for the binding of heavy nuclei, but it is not clear how much in error the calculation still may be.

If the second order calculation is tentatively accepted as substantially correct, one may investigate what slight modifications to the nuclear force could yield the observed binding. Two possibilities are considered. Firstly, the interaction effective in heavy nuclei may differ from that in light, owing to "many-body" forces. To represent this effect the magnitude of the potential has been increased, the parameters f and g of equation (4) being varied in the same proportion, while the meson mass, and hence $1/\lambda$, are left unaltered. The resulting energy per nucleon in an "ideal" nucleus, taken to be the minimum of $(\overline{T} + \overline{W} + E'')/A$ with respect to variation of size of the nucleus, is plotted against f^2 in Figure 2, curve (a). It will be seen that f^2 requires to be raised from the assumed value of 0.595 to 0.73—approximately 25% increase—to yield the observed binding. The corresponding predicted size of the nucleus, given by the r_0 which minimizes $(\overline{T} + \overline{W})$, is plotted against f^2 in Figure 2, curve (b). When f^2 is raised sufficiently to yield the correct binding, r_0 falls to 0.65, only about 75% of the observed value 0.85. Thus if many-body forces are invoked to account for the binding energy, the agreement regarding the size of the nucleus deteriorates.

Secondly, the interaction can be altered so as to yield the correct binding energy per nucleon in an "ideal" nucleus, by making this one of the quantities by which the parameters of the interaction (equation (4)) are fixed. The interaction can then be compatible with only two at most of the three quantities pertaining to light nuclei, by which the parameters were fixed by Fröhlich $et\ al.\ (1947)$: the two lowest levels of the neutron-proton system have been retained, while the ground-state energy of H^3 was abandoned. By fitting the two former quantities, f^2 and g^2

were calculated approximately for each value of the meson mass μ , a method differing only slightly from that of Fröhlich et al. (1947, §3) being employed. Then for each meson mass the binding energy per nucleon of an "ideal" nucleus was calculated, as shown in Figure 3, curve (a). Again, the minimum of $(\overline{T} + \overline{W} + E'')$ with respect to size of the nucleus was taken. It is found that to obtain the observed binding energy the mass of the meson required is 400m. The values of f^2 and g^2 appropriate to this meson mass are $f^2 = 0.60$, $g^2 = 0.11$.

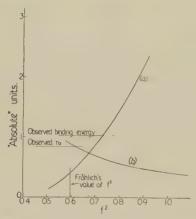


Figure 2. Effect of postulated "many-body" forces: change of binding energy and size of nucleus with effective nuclear-force parameter f^2 . Curve (a): Binding energy per nucleon by second order perturbation calculation, i.e. (-1)×minimum of

 $(\overline{T} + \overline{W} + E^{\prime\prime})/A$. Curve (b): Radius r_0 which minimizes the variation energy $(\overline{T} + \overline{W})$. To obtain observed binding energy, f^2 has to be raised from given value 0.595 to 0.73: the radius r_0 then falls to 0.65 (observed value 0.85).

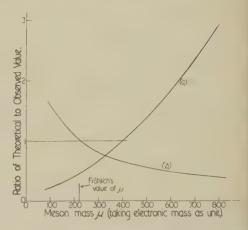


Figure 3. Predictions for heavy nucleus, when meson mass is variable, and interaction parameters are chosen to fit two observed constants of neutron-proton system.

Curve (a): Binding energy per nucleon by second order perturbation calculation, i.e. $(-1) \times mini$ mum of $(\overline{T} + \overline{W} + E'')/A$.

Curve (b): Radius r_0 which minimizes the variation energy $(\overline{T} + \overline{W})$.

To obtain observed binding energy, mass of meson must be 400m: r_0 then falls to 67% of observed value.

Together with each binding energy is found a prediction of the size of the nucleus (the value of r_0 minimizing (T+W)), which is shown plotted in Figure 3, curve (b). When the meson mass is 400m, r_0 is only $67^{\circ}_{/0}$ of the observed value. Thus, again, fitting of the binding energy is incompatible with correct nuclear size.

§ 3. CALCULATION OF THE BINDING ENERGY

3.1. Use of the Fermi-gas Model

On this model the nucleus is treated in the lowest approximation as an assembly of non-interacting particles, enclosed in a box at zero potential, with high potential walls. If the nucleons—neutrons and protons alike—are described by space, spin and isotopic coordinates, then the exclusion principle requires the wave function to be antisymmetric with respect to interchange of all the coordinates of any pair of particles. Suitable antisymmetric wave functions for the system may be built up in determinantal form from different individual wave functions for single particles. The composite wave functions so obtained will be approximate eigenfunctions for the system, provided the individual wave functions are given by

$$\Psi_r = \psi_l \omega_\mu.$$
(6)

 ψ_p is a function of the space coordinates only, zero outside the box, and

$$\psi_l = (8L^3)^{-\frac{1}{2}} \exp\left(\mathrm{i}(\mathbf{k}_{\rho}, \boldsymbol{\xi})\right) \qquad \dots (7)$$

inside the box. Here 2L is the length of the sides of the cube constituting the box, ξ is the space-coordinate of the particle concerned, \mathbf{k}_l is the dimensionless momentum, quantized by the condition

$$\mathbf{k}_l = \mathbf{n}_l \pi / L, \qquad \dots (8)$$

where \mathbf{n}_{ρ} is any vector whose components are all integers. ω_{μ} in equation (6) is one of the four spin and isotopic wave functions:

$$\omega_1 = \alpha \xi, \quad \omega_2 = \beta \xi, \quad \omega_3 = \alpha \eta, \quad \omega_4 = \beta \eta, \quad \dots$$
 (9)

where α and β are the Pauli spin wave functions, and ξ and η are similar for the isotopic coordinates.

To represent the ground state of the system, the composite wave function is built up of the A individual wave functions Ψ_r of lowest momentum k_l . For the "ideal" nucleus considered, the A/4 spatial wave functions ψ_l of lowest momentum are associated each in turn with all four ω_u .

The Fermi-gas model described has now to be used to calculate the groundstate energy of the system of nucleons with nuclear interactions operative.

In § 3.2 a variation calculation is performed, using the ground-state wave function of the model, together with the Hamiltonian of the "ideal" nucleus, to find

$$E = \overline{T} + \overline{W}, \qquad \dots (10)$$

where \overline{T} is the expectation kinetic energy, and \overline{W} the expectation potential energy. This is carried out initially for arbitrary dimension L of the box.

A perturbation approach is adopted in §3.3. Here the Fermi-gas of non-interacting particles is taken as an unperturbed system and the nuclear interaction W is applied as perturbation. The unperturbed energy is the kinetic energy \overline{T} , and the first order perturbation energy is \overline{W} , both already calculated. The second order approximation adds an energy E'', given by

$$E'' = -\sum_{R} |W_{0R}|^2 / (E_R^0 - E_0^0);$$
(11)

where the suffix R indicates the Rth unperturbed state and the suffix 0 the ground state. Σ' indicates summation over all states but the ground state, obtained by building the composite wave function from all possible combinations of different individual wave functions. The size chosen for the box is again initially arbitrary. The index 0 on the energy indicates the unperturbed kinetic energy of the state concerned.

3.2. Variation Method

The expectation kinetic energy \overline{T} is first calculated. In the dimensionless variables employed, it is found that

$$\overline{T} = -\frac{1}{2} \int \Phi^* \left(\sum_{s=1}^A \nabla_s^2 \right) \Phi dq = \frac{1}{2} \sum_{\text{states}} k_l^2, \qquad \dots (12)$$

where Φ is the ground-state wave function of the Fermi-gas model and $\int dq$ indicates integration or summation over all coordinates. The individual spatial states occupied form a lattice in **k** space, with a spacing π/L (cf. equation (8)). The occupied points, each four times occupied, are all those points falling within a sphere of radius a, given by

 $a = \frac{A^{\frac{1}{2}}}{2L} \left(\frac{3}{2}\pi^2\right)^{\frac{1}{2}} = \frac{(9\pi)^{\frac{1}{2}}}{r_0}.$ (13)

The sum in (12) can approximately be replaced by an integral in **k** space, evaluation of which yields

$$\overline{T}/A = 3a^2/10. \qquad (14)$$

The expectation potential energy is next found, using for the potential operator $\sum_{i < j} w_{ij}$, where w_{ij} is given by (4), and the same wave function Φ . The result is

$$\overline{W} = \frac{1}{2} \sum_{r,s} [(rs \mid w \mid rs) - (rs \mid w \mid sr)], \qquad \dots (15)$$

where, for instance,

$$(rs \mid w \mid rs) = \int \Psi_r^*(1) \Psi_s^*(2) w_{12} \Psi_r(1) \Psi_s(2) dq_1 dq_2$$

and the sum takes r and s over all occupied individual-nucleon states.

The matrix elements involved may be split into spatial and non-spatial parts if we write (cf. (4))

$$\Gamma_{ij} = (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_i)[g^2 + f^2(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_i)]; \qquad v_{ij} = \{\exp(-\xi_{ij})\}/\xi_{ij}, \quad \dots (16)$$

so that (15) becomes

$$\overline{W} = \frac{1}{2} \left\{ \left[\sum_{\mu,\nu=1}^{4} (\mu\nu | \Gamma| \mu\nu) \right] \left[\sum_{l,m} (lm|v|lm) \right] - \left[\sum_{\mu,\nu=1}^{4} (\mu\nu | \Gamma| \nu\mu) \right] \left[\sum_{l,m} (lm|v|ml) \right] \right\}.$$

$$\dots (17)$$

 μ , ν are non-spatial, and l, m are spatial quantum numbers (cf. equation (6)), the latter to be summed over the occupied sphere in \mathbf{k} space. The first, non-exchange, term vanishes, on account of the non-spatial factor, in conformity with the saturation requirements of nuclear forces (Rosenfeld 1948, chap. XI). Towards the evaluation of the remaining exchange term, it is found that

$$\sum_{\mu,\nu=1}^{4} (\mu\nu | \Gamma | \nu\mu) = 12(g^2 + 3f^2), \qquad \dots (18)$$

and

$$(lm |v| ml) = \frac{\pi}{2L^3} \frac{1}{1 + |\mathbf{k}_l - \mathbf{k}_m|^2}.$$
 (19)

The sum over l, m in (17) is replaced by a double integral in \mathbf{k} space, leading to the final result

$$\overline{W}/A = -(9/8\pi)(g^2 + 3f^2)\Omega_1(a),$$

where

$$\Omega_1(a) = 2\left[\frac{1}{2a} + \frac{1}{3(2a)^3}\right] \ln\left(1 + (2a)^2\right) + \left(2a - \frac{2}{3}\frac{1}{2a}\right) - \frac{8}{3}\tan^{-1}(2a). \quad \dots (20)$$

The kinetic and potential energies of equations (14) and (20) are plotted against r_0 in Figure 1, curves (a) and (b), for the values of f^2 and g^2 given in equation (5).

3.3. Second Order Perturbation

The second order contribution to the energy (equation (11)) requires evaluation of the matrix element W_{0R} for each excited, unperturbed state R. The only states giving non-zero contributions are those built up from a set of individual wave functions Ψ_r and differing only by one or two constituents from the set constituting the ground state; and of these, the only ones which may not be neglected are those obtained from the ground state by replacing two individual wave functions Ψ_r , Ψ_s by two others $\Psi_{r'}$, $\Psi_{s'}$ satisfying a "conservation of momentum" condition

$$\mathbf{k}_l + \mathbf{k}_m = \mathbf{k}_{l'} + \mathbf{k}_{m'}, \qquad \dots (21)$$

where l, m etc. are the spatial quantum numbers pertaining to the individual states r, s, etc. respectively (cf. equation (6)). Development of (11) then yields

$$E'' = -\sum_{r,s} \sum_{r',s'} \frac{|(rs|w|r's')|^2 - (rs|w|r's')^*(rs|w|s'r')}{(k_{l'}^2 + k_{m'}^2) - (k_l^2 + k_m^2)}. \quad \dots (22)$$

Here Σ means double summation over all ground-state constituent individual states Ψ_r and Ψ_s , and Σ' means double summation over all the other individual states $\Psi_{r'}$ and $\Psi_{s'}$ conforming to the selection rule (21). The spatial and non-spatial factors in the matrix elements are now separated out, as in the previous subsection. The sum over the non-spatial quantum numbers involved is readily carried out, with the result

$$E'' = -\sum_{l,m} \sum_{l',m'} \frac{A \left| (lm \mid v \mid l'm') \right|^2 - B(lm \mid v \mid l'm')^* (lm \mid v \mid m'l')}{(k_{l'}^2 + k_{m'}^2) - (k_l^2 + k_m^2)}, \quad \dots (23)$$

where $A = 48(g^4 + 3f^4)$, $B = 12(3f^4 - 6g^2f^2 - g^4)$. The spatial quantum numbers l, m are each to be summed over the sphere of radius a in \mathbf{k} space; and l', m' are each to be summed over the space exterior to this sphere, subject to the selection rule (21).

Evaluation of (lm | v | l'm') yields

$$(lm | v | l'm') = \frac{\pi}{2L^3} \frac{1}{1 + \frac{1}{4} |\mathbf{k}_{l'} - \mathbf{k}_{l} - \mathbf{k}_{m'} + \mathbf{k}_{m}|^2} \cdot \dots (24)$$

The sums in (23) may, as usual, be replaced by integrals in \mathbf{k} space. By an obvious abbreviation, (23) may be written

$$E'' = -(AI - BJ). \qquad \dots (25)$$

It has been found possible to evaluate I but not J. However, it appears that the intractable term containing J is negligible; for it readily follows from the form of the integrals that I > J > 0, and insertion in (23) of the values of f^2 and g^2 given in (5) shows that $|A| \gg |B|$, in fact A = 217, B = 3.6.

Thus neglect of the term BJ introduces an error of less than 2%. The smallness of the error is to some extent due to fortunate given values of f^2 and g^2 : it may be noted, however, that the form of A and B is such that the error could not exceed -25% to +50% for any values of f^2 and g^2 whatever.

Evaluation of I from (23) and (24) then yields finally

$$E''/A = (-9/2\pi^2)(g^4 + 3f^4)\Omega_2(a),$$

where

$$\Omega_{2} = \ln\left(1 + (2a)^{2}\right) \cdot \left[\frac{13}{12} - \frac{4}{3}\ln 2 + \frac{1}{4(2a)^{2}}\right] - \frac{7}{18} + \frac{49}{18}\ln 2 + \frac{5}{6}\ln 2 \cdot \frac{1}{(2a)^{2}} \\
+ \cot^{-1}\left(2a\right) \left[2a - \frac{2}{3}\frac{1}{2a}\right] + \left[\frac{1}{2}(2a) + \frac{1}{2a} + \frac{1}{2}\frac{1}{(2a)^{3}}\right] \int_{0}^{\tan^{-1}(2a)} \ln\left(2\cos x\right) dx \\
+ 2\left[1 + \frac{1}{3}\frac{1}{(2a)^{2}}\right] \int_{0}^{1} \frac{\ln\left(1 - x^{2}\right)}{x^{2} + (2a)^{2}} dx - \frac{8}{3}(2a)^{2} \int_{0}^{1} \frac{\tanh^{-1}x}{x(x^{2} + (2a)^{2})} dx \cdot \dots (26)$$

This is plotted against r_0 in Figure 1, curve (d), for the f^2 and g^2 of equation (5).

§ 4. CRITICISM OF CALCULATIONS

The argument has proceeded by the three following stages, each of which requires to be examined: (i) by a semi-empirical approach, based on equation (1), the binding energy per nucleon of an "ideal" nucleus has been determined; (ii) the parameters in the nuclear force employed have been chosen to fit certain properties of light nuclei; (iii) the nuclear force has been used to calculate approximately the binding energy per nucleon of an "ideal" nucleus, for comparison with the result of (i).

The procedure of the first stage is well known, and an extensive literature (e.g. Bethe and Bacher 1936, § 30, Mattauch and Flügge 1942, p. 90, Feenberg 1947) establishes that the results obtained for the "ideal" nucleus can be relied upon to the accuracy relevant here.

Stage (ii) was carried out by Fröhlich et al. (1947), and is again probably sufficiently accurate as a basis for the present calculations.

Stage (iii) concerns the accuracy of the approximate solutions of the Schrödinger equation. The inadequacy of the variation calculation is palpable, in view of the relative largeness of the second order perturbation result. As regards the latter, it may be noted that, even if high order perturbation energies were calculated, and if they converged, the Fermi-gas model could only yield the energy of the system of particles when enclosed in a box of the assumed size, with infinitely high walls. The method is thus best considered as an approximation to a solution for the nucleus so immured. For each order of perturbation, the best energy would be taken as the minimum with respect to variation of the size of the box. From this viewpoint, three orders of perturbation energy have been obtained, viz. \overline{T} , \overline{W} and E''. The only available criterion of the goodness of the approximation is the rate of apparent convergence of these terms; per nucleon, they are in order (for the interaction parameters assumed, and at the radius which minimizes their sum) 1.35, -1.41, -0.35 (sum = -0.41) (in absolute units). These figures might suggest inception of convergence, but only at a slow rate.

§ 5. SVARTHOLM VARIATION-ITERATION METHOD

The method developed by Svartholm (1945) has been used by him to investigate the ground states of the lightest nuclei, and its application to heavier nuclei seemed worth considering. It is found, however, that the method loses its usual advantage of assured convergence in such an application; and in practice a calculation with the Fermi-gas model has yielded no useful results.

The convergence question will be dealt with first. Reference should be made to Svartholm's thesis (1945) for an account of the method, but it may be remarked

here that by an iteration procedure one may obtain in principle a succession of approximations $\Lambda_0, \Lambda_1, \ldots$ to the eigenvalue Λ of the interaction constant required to yield a given binding energy. A virtue of the method is that, subject to certain conditions, the series of approximations $\Lambda_0, \Lambda_1, \ldots$ decreases monotonically towards the required eigenvalue. One of those conditions, however, is that the potential function u should be "negative definite", i.e. for any arbitrary wave function Φ , $\int \Phi^* u \Phi dq \leqslant 0$. Now one requirement of a nuclear force suitable for heavier nuclei is that it shall lead to the "saturation" phenomenon (Rosenfeld 1948, chap. XI), and it can be shown very generally that this implies that the potential shall *not* be negative definite. Thus for such a force, there is in general no assurance of the convergence of the series of approximations.

Nevertheless, the author has made a calculation with the method, using as initial wave function the Fermi-gas function of § 3.1. The zero-order calculation yielding Λ_0 , is then simply equivalent to the variation treatment of § 3.2. $\Lambda_{\frac{1}{2}}$ was next calculated, only leading terms with respect to powers of A being retained. The result found was that, quite generally, for any type of saturating short-range potential, $\Lambda_{\frac{1}{2}}$ is identically the same as Λ_0 . Thus to this order, the Svartholm treatment gives no improvement over the variation treatment.

ACKNOWLEDGMENT

The author is happy to express his sincere thanks to Dr. H. Fröhlich, who suggested this subject, and has been unsparing of advice and encouragement.

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REVIEWS OF BOOKS

Practical Five-figure Mathematical Tables, by C. Attwood. Pp. v+74. (London: Macmillan and Co. Ltd., 1948.) 3s.

The publication of this set of tables is an event of more importance than would at first meet the eye. The first mathematical tables were naturally of many figures, and then, in the nineteenth century, logarithmic and trigonometric tables settled down to seven figures as the norm. Towards the end of the century, and for the first part of the twentieth, the value of four-figure tables for the scientist was realized, and many a set was issued. With them, were a few six-figure sets and a fair number of five-figure ones. But their compilers followed each other rather monotonously, and seldom introduced real innovations, except for a few impracticable ones. The present reviewer, for example, has (or has lent and lost), more than a dozen different books of four or five figure compilations, most of them indistinguishable from each other.

The difference that marks this, and that ought to make it very widely known and used, is that the author has thought out afresh what functions are wanted, at what intervals they

should be tabulated, and the most convenient means for interpolation in them,

His choice of functions does not in fact offer any surprises. There are no transcendental functions such as we find in Dale's five-figure tables, or in Jahnke and Emde, but a generous selection of those likely to be wanted in an all-purpose compilation. Logarithms and anti-logarithms, the six trigonometric functions, both natural and logarithmic, for degrees and minutes, we may take for granted. In addition, Mr. Attwood gives us logarithms of reciprocals (to save subtraction) and trigonometric functions of angles given in radians; he also tabulates squares and square roots, cubes and cube roots, the fourth and fifth roots of integers to 100, and the exact values of powers up to the sixth of integers from 1 to 100, as well as reciprocals. Then there are natural logarithms and exponential functions and (a concession to engineers?) the areas of circles.

Logarithms and trigonometrical functions offer difficulties in places, as we all know, where they change rapidly, and there are many ways in use for turning the difficulty. We may use the reciprocal or the function of the complement of the angle, or we may tabulate some function which varies less rapidly, we may vary the interval of the argument, or we may use the inverse function. Mr. Attwood points out, at the appropriate page, when the former expedients are desirable, but in general he relies on the method of changing the interval. This he has done most judiciously. Related to this matter is the question of the use of proportional parts: some five-figure tables give proportional parts in little marginal tables. leaving the user to form his own differences and to take the appropriate proportional parts (the reviewer's favourite five-figure tables, due to Schlömilch, take them to one extra decimal place and indicate whether the tabular entries are in excess or defect, so that there is no loss of accuracy) whilst others give mean proportional parts applicable to a whole line of the table. These are dangerous when the differences change rapidly, and it is not uncommon to give two lines of mean proportional parts, splitting the tabular entries to share them between the two. In the present volume, this device is widely adopted and somewhat extended, so that as many as four lines of mean proportional parts (m.p.p.) may be given to a line of the table. The m.p.p. have been individually examined to get the best compromise, and are printed in red whenever they have to be subtracted. The author asserts that more than 95% of the 160.533 combinations obtainable with the m.p.p. are in error by 0 or 1 unit, only 0.6%leading to errors of more than 3 units. Where there is a danger of error of five units, the m.p.p. are in italics, so that a user can use proper interpolation methods if needed. There is a table showing the maximum possible error in every table, but here the author is unfair to himself. No one could use m.p.p. to stretch across more than half the tabular interval, but should always take differences from the nearest entry. This would reduce the errors in a number of places. Where m.p.p. are not given, the user is instructed to adopt linear or second-difference interpolation, and is given instruction in this, with a critical table of Bessel coefficients, but second differences are never printed as part of the tables.

To close with a few words on general points. The author has varied in his interpretation of five figures. In some tables, it means five decimal places, as in the cosine of 89° 42′, which is 0.00524, and sometimes five significant figures, as in the secant of the same angle, which is 190.99. From the latter, with the aid of the table of reciprocals, we may find that the cosine is really 0.0052359, or from the tables of logarithmic cosines and antilogs, we may find it as 0.0052360. In the table of secants, there is a change at 45° from five decimal to five significant figures.

The printing is good, and there is a strong limp cloth cover. If any change in a good book might be suggested, it is a thumb index to enable two tables to be used in conjunction more easily. To find out if there are misprints will call for longer use, or for deliberate and systematic examination of differences.

J. H. A.

Some Aspects of the Luminescence of Solids, by F. A. Kröger. Pp. xii + 310. (New York and Amsterdam: Elsevier Publishing Co., 1948.) \$5.50 (30s.).

The luminescence of solids is a subject which has benefited much from the development of theoretical conceptions of the solid state during the last fifteen years; perhaps before long we shall see new theoretical ideas arising as a result of new experimental work. The work of the Lenard School during the early years of the century was the most significant in this field, but, unfortunately, the lack of a satisfactory theoretical picture of the behaviour of electrons in solids robbed much of the work of the value it might otherwise have had.

During the last ten years a great deal of attention has been given to the study and understanding of afterglow or phosphorescence phenomena in solids, and there have been notable advances. While to some extent a reasonably satisfactory picture can now be given of these effects, we know little as yet about the nature of luminescence centres and electron traps in solids. These problems in relation to infra-red sensitive phosphors and their properties are particularly important, and it is in this direction that we may hope for new advances.

Dr. Kröger's volume is of a rather special category, in that it is a research monograph and not a comprehensive review of a wide field of work. The volume is based on experimental work carried out in the physics laboratories of the N. V. Philips Gloeilampenfabrieken, Eindhoven, during the last five years, or it may be assumed that it represents a convenient form of publication of work carried out during, and held up by, the war.

The first chapter contains a useful account of energy levels in pure and perturbed crystals, and an attempt is made to develop a general picture capable of covering all possible luminescent effects. Some of us will think that it is a little early for such attempts, but are

nevertheless grateful for the setting out of Dr. Kröger's ideas in coherent form.

In the following four chapters the author discusses new experimental results on tungstates, molybdates and phosphors activated by manganese, titanium and uranium. In the final chapter the effect of temperature on the efficiency of luminescence has been considered. The data presented in these chapters will be of value to other workers in the subject, but can hardly be expected to interest a wider audience. The book ends with 36 pages of tabular matter of the kind only too familiar to readers of Vol. XXIII/1 of the Handbuch der Experimental Physik. Is it of much scientific value to be told that the luminescence of magnesium orthosilicate is "violet"? Or that the luminescence is "strong" or "weak" or "faint"? I think not: it is time for workers and writers in this field to rid themselves of these older inexact traditions if the subject is to advance as it should. Dr. Kröger's volume is a useful addition to the research literature of the luminescence of solids, and the work described must, for the most part, have been carried out under appallingly difficult conditions.

J. T. RANDALL.

Electrons and Nuclear Counters, by S. A. Korff. Pp. xi+212. (New York and Toronto: D. Van Nostrand Co. Inc., 1947; British Agents: Macmillan and Co. Ltd., London.) 18s. net.

Until a few years ago, an aura of mystery surrounded the mode of operation of a Geiger-Müller counter and it was regarded as an erratic device which had to be made according to some favourite "cookery-book" recipe. Recent advances in our knowledge of the discharge mechanism in these counters has done much to clarify the situation so that they are now standard tools for work on nuclear physics and are being satisfactorily manufactured commercially. There has been a deeply felt need for a book giving an up-to-date account of the state of the subject and Professor Korff is to be congratulated upon a pioneer effort on these lines.

It should perhaps be stated at the outset that he has produced a survey suitable for the student and general reader rather than a work of reference for the specialist. The book opens with an introductory chapter describing the different modes of operation of an ion counter, that is, its use as an ionization chamber, proportional counter or Geiger-Müller counter. The next three chapters, which form the main body of the book, discuss each of these modes of operation in more detail, the main stress being laid on the Geiger-Müller region. The fundamental principles involved are well brought out and a good general account is given of the discharge which occurs in the gas of the counter and of the various factors which influence it. Unfortunately this account suffers from a rather poor arrangement of the material so that there is a considerable amount of repetition and frequent and very irritating references forward to matters dealt with subsequently.

In chapter five, the author gives a very clear account of the principles and procedure involved in the practical construction of counters. He has dealt only with the cylindrical cathode, axial-wire anode type of counter. Sections dealing with other types, such as point counters and parallel plate ionization chambers would have been valuable additions. There

follows a brief chapter on the errors and corrections involved in counting. The treatment is rather sketchy and can only be regarded as a general introduction to the subject. The final chapter deals with some of the auxiliary electronic circuits employed in conjunction with counters. This constitutes a very extensive subject in itself, so that, in the space at his disposal, the author has been able to give only a very brief outline of the types of circuits which can be employed. The book also includes a fairly comprehensive list of references to original papers on ion counters. Summing up, Professor Korff's book can be recommended to those readers who want a good general introduction to the behaviour of ion counters.

J. L. MICHIELS.

Theoretical Aerodynamics, by L. M. MILNE-THOMSON, M.A., F.R.S.E. Pp. xx+363. (London: Macmillan & Co., 1948.) 40s.

The purpose for which this book is written is to give a sound mathematical basis of theoretical aerodynamics on which applications to practical problems of aircraft design and flight must rest and to state clearly the underlying assumptions of the mathematical theory so that there is no uncertainty on what can legitimately be deduced from the assumptions

as a first approximation.

The book has 19 chapters. Chapters I and II are introductory and concerned mainly with general features of fluid motion. Chapters III to XII and Chapter XIV deal in a commendable manner with well-known subjects of theoretical aerodynamics, namely two-dimensional motion, rectilinear vortices, the properties of two-dimensional airflow past a circular cylinder, Joukowski's transformation theory of two-dimensional aerofoils, thin aerofoils, induced velocity, aerofoils of finite aspect ratio, lifting-line theory, lifting-surface theory and wind-tunnel corrections. The treatment of the mathematical theorems and of the illustrative applications chosen is made as simple as possible to help a reader whose mathematical knowledge does not extend much beyond the elements of the differential and integral calculus. The appeal which the selected applications make to an aerodynamicist familiar with the subject will depend on the extent to which his needs have been appreciated by the author: but the illustrations chosen give clues for the solution of related applications.

Chapter XV on subsonic and supersonic flow serves as an introduction to a subject on which a great deal of theoretical investigation has been made during recent years. Present knowledge on the mathematical theory of compressible flow is sufficient to provide subject matter for a complete book: it is not to be expected that it could be treated adequately in a single chapter. Chapter XIII and Chapters XVI–XVIII on propellers, simple flight problems, moments and aircraft stability respectively are limited in scope but suffice to give a student an insight into some theoretical problems related to the performance and behaviour of aircraft. Chapter XIX is well worth inclusion for the benefit of a reader who has little or no acquaintance with vector methods of presentation.

Exercises for a student are given at the end of each chapter: lists of references to relevant papers are unfortunately not given. It is perhaps surprising that a chapter on the mathematical theory of boundary-layer flow is not included.

The book fulfils the purpose for which it was written: it can be recommended as a good introduction to theoretical aerodynamics.

A. FAGE.

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ABSTRACTS FOR SECTION B

On the Theory of Aplanatic Aspheric Systems, by G. D. WASSERMANN and E. Wolf.

ABSTRACT. Methods are described for the design of two aspheric surfaces for any given centred system, so as to achieve exact aplanatism. The practical application of the methods is illustrated by the design of a reflecting microscope.

The Refractive Index in Electron Optics and the Principles of Dynamics, by W. Ehrenberg and R. E. Siday.

ABSTRACT. In view of mis-statements made in the literature, the origin of the refractive index in electron optics is discussed in some detail, and the uniqueness of an expression previously given is demonstrated. On this basis, some general properties of electron optics are investigated.

A relation between ray direction and wave normal is obtained. Whereas the refractive index is unique in terms of the magnetic vector potential **A**, this itself is arbitrary to some extent. It is shown that **A** must, for purposes of electron optics, be chosen so as to satisfy Stokes' theorem and that, if it does, no observable effects result from the arbitrariness of **A**. An expression for the optical path difference is given in terms of the magnetic flux enclosed. The results are applied to a number of questions, viz. the differential equations for trajectories, the focusing properties of an axially symmetric field and the interference pattern produced by two converging bundles of rays which enclose a magnetic flux.

The Disturbance near the Focus of Waves of Radially Non-Uniform Amplitude, by H. H. HOPKINS.

ABSTRACT. Lommel's problem, the disturbance near the focus of waves of uniform amplitude, is generalized to consider waves of radially non-uniform amplitude. Lommel's numerical results are extended, and his U and V functions, tabulated on a new basis, together with some new related functions, are employed to provide extensive intensity distribution curves for the diffracting patterns associated with waves of both uniform and non-uniform amplitude.

Some Spectroscopic Observations on Pyrotechnic Flames, by R. F. Barrow and E. F. Caldin.

ABSTRACT. The results of a spectroscopic study of the white or coloured flames from typical pyrotechnic compositions are reported. Most of the visible light from these sources comes from a limited number of atomic or diatomic emitters. The effects of secondary emitters on the dominant wavelength, colorimetric purity and relative intensity are considered in general terms and some suggestions for improving the quality of the flames are put forward.

Some Experiments on Photo-ionization in Gases, by A. A. JAFFE, J. D. CRAGGS and C. BALAKRISHNAN.

ABSTRACT. From an investigation of the discharge spread in Geiger counters filled with hydrogen, neon, argon or helium, it is possible to show that in certain circumstances the discharge spread is due almost entirely to photo-ionization in the gaseous counter filling. The results enable the absorption coefficients of the operative radiations to be found.

The Excitation and Transport of Metal Vapour in Short Sparks in Air, by G. C. WILLIAMS, J. D. CRAGGS and W. HOPWOOD.

ABSTRACT. The paper describes a study of the excitation temperature in certain spark discharges of accurately known current characteristics. The excitation temperatures are found by measuring intensity ratios for certain spectral lines where the relevant transition probabilities are known, and are compatible with earlier work by Ornstein and his collaborators on arc discharges.

The excitation temperatures are, as would be expected, higher than those generally found for arc conditions.

Certain peculiarities relating to the evaporation of electrode metal are described. In particular the presence of discontinuous evaporation was noticed, and it was found that different electrode metals showed considerable variations in their behaviour in this respect.

Measurements on the Velocity of Sound in Mixtures of Hydrogen, Helium, Oxygen, Nitrogen and Carbon Monoxide at Low Temperatures, by A. VAN ITTERBEEK and W. VAN DONINCK.

ABSTRACT. Values of the velocity of sound in H₂-N₂, H₂-O₂, H₂-CO, He-N₂, He-O₂ mixtures of varying proportions have been determined by experiment and compared with the theoretical values. Curves showing the variation of sound velocity with the pressure of the mixtures for different temperatures (65° K, to 90° K,) are given.

Ultrasonic Dispersion in Organic Liquids, by A. Schallamach.

ABSTRACT. The sound velocities v have been measured, at frequencies f between about 700 and 3,000 kc/s., and at temperatures between about $\pm 15^{\circ}$ and -80° c., of the following liquids: geraniol, di-dihydrocitronellyl ether, castor oil and iso-butyl alcohol. There is evidence of a positive dispersion $(\partial v/\partial f>0)$ in the first three liquids at low temperatures. A negative dispersion has been observed in geraniol and di-dihydrocitronellyl ether at higher temperatures, and in iso-butyl alcohol over the whole temperature range.

The positive dispersions are discussed on the basis of the classical hydrodynamic theory, and the implications of a complex viscosity are examined.

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